

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSSPTA1626GMS

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * Welcome to STN International * * * * *

NEWS 1 Web Page URLs for STN Seminar Schedule - N. America
NEWS 2 "Ask CAS" for self-help around the clock
NEWS 3 FEB 28 PATDPAFULL - New display fields provide for legal status
data from INPADOC
NEWS 4 FEB 28 BABS - Current-awareness alerts (SDIs) available
NEWS 5 MAR 02 GBFULL: New full-text patent database on STN
NEWS 6 MAR 03 REGISTRY/ZREGISTRY - Sequence annotations enhanced
NEWS 7 MAR 03 MEDLINE file segment of TOXCENTER reloaded
NEWS 8 MAR 22 KOREAPAT now updated monthly; patent information enhanced
NEWS 9 MAR 22 Original IDE display format returns to REGISTRY/ZREGISTRY
NEWS 10 MAR 22 PATDPASPC - New patent database available
NEWS 11 MAR 22 REGISTRY/ZREGISTRY enhanced with experimental property tags
NEWS 12 APR 04 EPFULL enhanced with additional patent information and new
fields
NEWS 13 APR 04 EMBASE - Database reloaded and enhanced
NEWS 14 APR 18 New CAS Information Use Policies available online
NEWS 15 APR 25 Patent searching, including current-awareness alerts (SDIs),
based on application date in CA/CAPLUS and USPATFULL/USPAT2
may be affected by a change in filing date for U.S.
applications.
NEWS 16 APR 28 Improved searching of U.S. Patent Classifications for
U.S. patent records in CA/CAPLUS
NEWS 17 MAY 23 GBFULL enhanced with patent drawing images
NEWS 18 MAY 23 REGISTRY has been enhanced with source information from
CHEMCATS
NEWS 19 JUN 06 The Analysis Edition of STN Express with Discover!
(Version 8.0 for Windows) now available
NEWS 20 JUN 13 RUSSIAPAT: New full-text patent database on STN
NEWS 21 JUN 13 FRFULL enhanced with patent drawing images
NEWS 22 JUN 27 MARPAT displays enhanced with expanded G-group definitions
and text labels
NEWS 23 JUL 01 MEDICONF removed from STN
NEWS 24 JUL 07 STN Patent Forums to be held in July 2005
NEWS 25 JUL 13 SCISEARCH reloaded
NEWS 26 JUL 20 Powerful new interactive analysis and visualization software,
STN AnaVist, now available
NEWS 27 AUG 11 Derwent World Patents Index(R) web-based training during
August
NEWS 28 AUG 11 STN AnaVist workshops to be held in North America

NEWS EXPRESS JUNE 13 CURRENT WINDOWS VERSION IS V8.0, CURRENT
MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
AND CURRENT DISCOVER FILE IS DATED 13 JUNE 2005

08/16/2005 10635294.trn

NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS INTER	General Internet Information
NEWS LOGIN	Welcome Banner and News Items
NEWS PHONE	Direct Dial and Telecommunication Network Access to STN
NEWS WWW	CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

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* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 09:22:09 ON 16 AUG 2005

=>

Uploading

THIS COMMAND NOT AVAILABLE IN THE CURRENT FILE

Do you want to switch to the Registry File?

Choice (Y/n):

Switching to the Registry File...

Some commands only work in certain files. For example, the EXPAND command can only be used to look at the index in a file which has an index. Enter "HELP COMMANDS" at an arrow prompt (=>) for a list of commands which can be used in this file.

=> FILE REGISTRY

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 09:22:20 ON 16 AUG 2005

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

COPYRIGHT (C) 2005 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 15 AUG 2005 HIGHEST RN 860345-00-2

DICTIONARY FILE UPDATES: 15 AUG 2005 HIGHEST RN 860345-00-2

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

*
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *

08/16/2005 10635294.trn

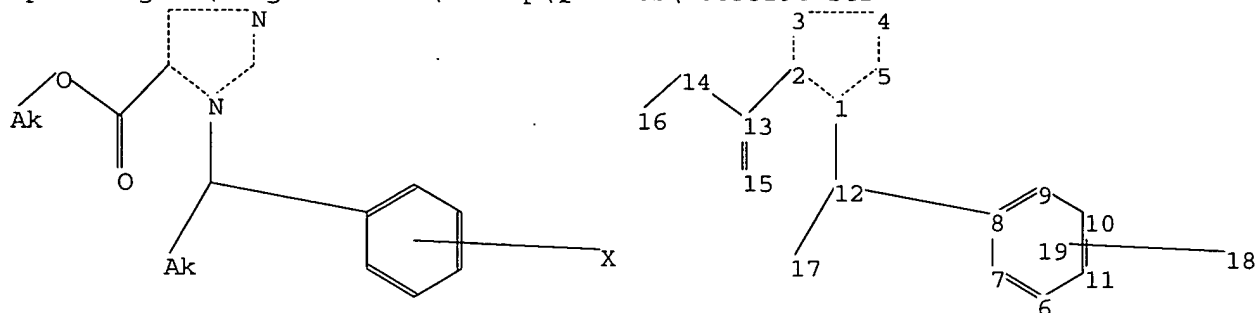
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
*

Structure search iteration limits have been increased. See HELP SLIMITS
for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10635294.str



chain nodes :

12 13 14 15 16 17 18

ring nodes :

1 2 3 4 5 6 7 8 9 10 11

chain bonds :

1-12 2-13 8-12 12-17 13-14 13-15 14-16

ring bonds :

1-2 1-5 2-3 3-4 4-5 6-7 6-11 7-8 8-9 9-10 10-11

exact/norm bonds :

1-2 1-5 1-12 2-3 3-4 4-5 12-17 13-14 13-15 14-16

exact bonds :

2-13 8-12

normalized bonds :

6-7 6-11 7-8 8-9 9-10 10-11

isolated ring systems :

containing 1 : 6 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS
19:CLASS

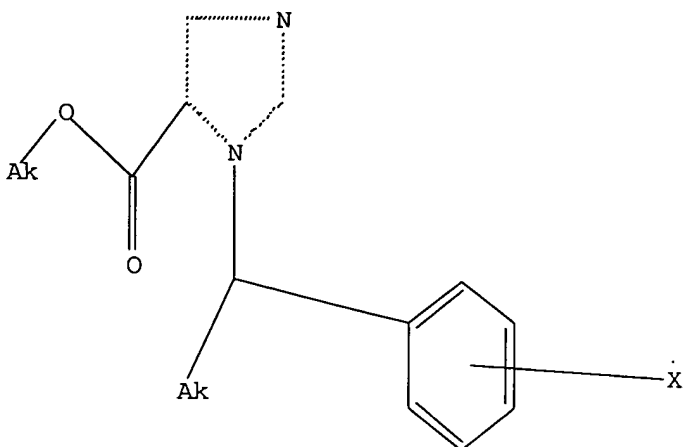
L1 STRUCTURE UPLOADED

08/16/2005 10635294.trn

=> d l1

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 09:22:36 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 452 TO ITERATE

100.0% PROCESSED 452 ITERATIONS

7 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 7765 TO 10315

PROJECTED ANSWERS: 7 TO 298

L2 7 SEA SSS SAM L1

=> s l1 sss full

FULL SEARCH INITIATED 09:22:43 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 9048 TO ITERATE

100.0% PROCESSED 9048 ITERATIONS

SEARCH TIME: 00.00.01

95 ANSWERS

L3 95 SEA SSS FUL L1

=> FIL HCAPLUS

~~COST IN U.S. DOLLARS~~

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

161.33

161.54

FILE 'HCAPLUS' ENTERED AT 09:22:48 ON 16 AUG 2005

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FILE COVERS 1907 - 16 Aug 2005 VOL 143 ISS 8
FILE LAST UPDATED: 15 Aug 2005 (20050815/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 13

L4 15 L3

=> FIL REGISTRY

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
9.80	171.34

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 09:25:22 ON 16 AUG 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 15 AUG 2005 HIGHEST RN 860345-00-2
DICTIONARY FILE UPDATES: 15 AUG 2005 HIGHEST RN 860345-00-2

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

*
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
*

Structure search iteration limits have been increased. See HELP SLIMITS for details.

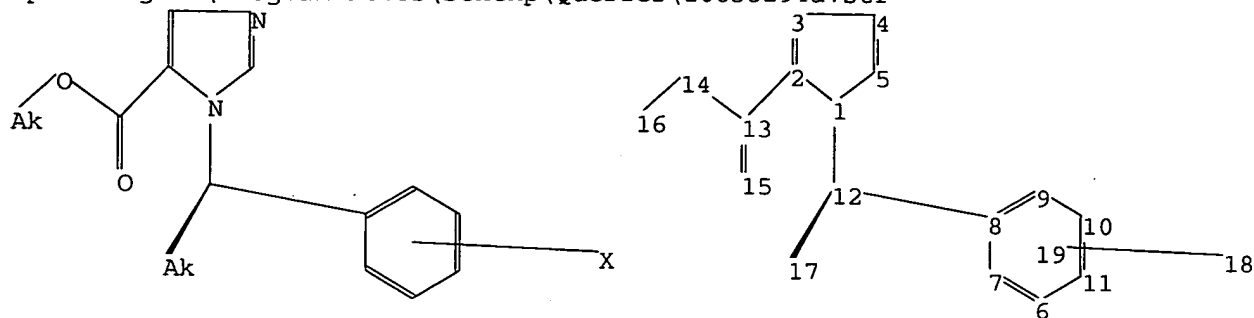
Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:

08/16/2005 10635294.trn

<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10635294a.str



chain nodes :

12 13 14 15 16 17 18

ring nodes :

1 2 3 4 5 6 7 8 9 10 11

chain bonds :

1-12 2-13 8-12 12-17 13-14 13-15 14-16

ring bonds :

1-2 1-5 2-3 3-4 4-5 6-7 6-11 7-8 8-9 9-10 10-11

exact/norm bonds :

1-2 1-5 1-12 3-4 4-5 12-17 13-14 13-15 14-16

exact bonds :

2-3 2-13 8-12

normalized bonds :

6-7 6-11 7-8 8-9 9-10 10-11

isolated ring systems.:

containing 1 : 6 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom

11:Atom 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS

19:CLASS

Stereo Bonds:

17-12 (Single Wedge).

Stereo Chiral Centers:

12 (Parity=Don't Care)

Stereo RSS Sets:

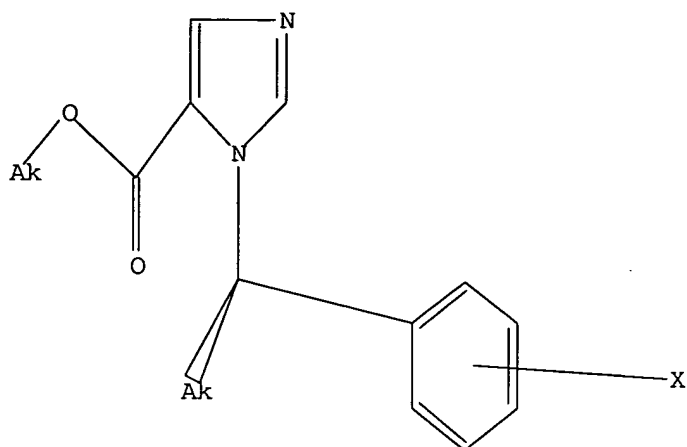
Type=Relative (Default). 1 Nodes= 12

L5 STRUCTURE UPLOADED

=> d 15

08/16/2005 10635294.trn

L5 HAS NO ANSWERS
L5 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l5
SAMPLE SEARCH INITIATED 09:25:40 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 452 TO ITERATE

100.0% PROCESSED 452 ITERATIONS 1 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 7765 TO 10315
PROJECTED ANSWERS: 1 TO 80

L6 1 SEA SSS SAM L5

=> s l5 sss full
FULL SEARCH INITIATED 09:25:46 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 9048 TO ITERATE

100.0% PROCESSED 9048 ITERATIONS
SEARCH TIME: 00.00.01

L7 19 SEA SSS FUL L5

=> FIL HCAPLUS
COST IN U.S. DOLLARS

SINCE FILE TOTAL
ENTRY SESSION
161.33 332.67

FULL ESTIMATED COST

FILE 'HCAPLUS' ENTERED AT 09:25:53 ON 16 AUG 2005
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19 ANSWERS

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FILE COVERS 1907 - 16 Aug 2005 VOL 143 ISS 8
FILE LAST UPDATED: 15 Aug 2005 (20050815/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 17

L8

6 L7

=> d his

(FILE 'HOME' ENTERED AT 09:22:09 ON 16 AUG 2005)

FILE 'REGISTRY' ENTERED AT 09:22:20 ON 16 AUG 2005

L1 STRUCTURE UPLOADED

L2 7 S L1

L3 95 S L1 SSS FULL

FILE 'HCAPLUS' ENTERED AT 09:22:48 ON 16 AUG 2005

L4 15 S L3

FILE 'REGISTRY' ENTERED AT 09:25:22 ON 16 AUG 2005

L5 STRUCTURE UPLOADED

L6 1 S L5

L7 19 S L5 SSS FULL

FILE 'HCAPLUS' ENTERED AT 09:25:53 ON 16 AUG 2005

L8 6 S L7

=> d 14 ibib abs hitstr tot

L4 ANSWER 1 OF 15 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2005:123220 HCAPLUS

DOCUMENT NUMBER: 142:198079

TITLE: Preparation of radiolabeled 1-(phenylethyl)imidazole-5-carboxylic acid ester derivatives

INVENTOR(S): Zolle, Ilse; Hammerschmidt, Friedrich

PATENT ASSIGNEE(S): Austria

SOURCE: U.S. Pat. Appl. Publ., 15 pp.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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US 2005033060 A1 20050210 US 2003-635294 20030806
 PRIORITY APPLN. INFO.: ~~20050210~~ US 2003-635294 20030806
 OTHER SOURCE(S): MARPAT 142:198079
 GI

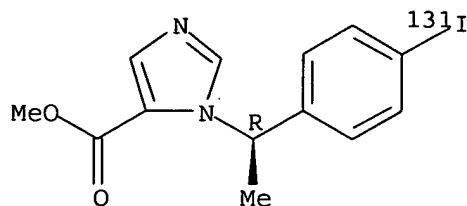
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Halogenated carboxylic ester derivs. of phenylethylimidazole (I) [R1 = linear or branched C1-4 alkyl which is optionally substituted with a halogen selected from the groups consisting of F, Cl, I or Br; R2 = C1-2 alkyl; X = a nonradioactive or a radioactive halogen] or (II) [X = a nonradioactive or radioactive halogen selected from the group consisting of I, Br, and F; X = a radioactive halogen selected from the group consisting of ¹²³I, ¹²⁴I, ¹³¹I, ⁷⁶Br, ⁸²Br or ¹⁸F] are prepared via coupling of (S)-secondary alc. (III) (R2, X = same as above) with imidazolecarboxylate ester (IV) (R1 = same as above). Radio-halogenated forms of these compds. are ideally suited for positron-imaging of the adrenal glands, as it is known that these compds. demonstrate a selective and high rate of accumulation in the adrenals. The method of preparing these derivs. proceeds by the conversion of a stable, non-radioactive intermediate having trialkylstannyl leaving groups (V) [R1, R2 = same as above; L = an alkylstannyl group selected from the group consisting of trimethylstannyl, triethylstannyl, tri-n-propylstannyl and tri-n-butylstannyl] and (VI) (R1, R2 = same as above). These intermediates are efficiently converted to the corresponding halogenated forms by substitution of the trialkylstannyl group with the halogen or radiohalogen. Thus, 4-iodoacetophenone was reduced by DIBAH in toluene/Et2O at -78° to give 86% 1-(4-iodophenyl)ethanol which was esterified by chloroacetic anhydride in the presence of pyridine in CH2Cl2 at 0° for 2 h to give 91% 1-(4-iodophenyl)ethyl chloroacetate (VII). VII underwent enzymic hydrolysis in the presence of lipase SAM II in a mixture of tert-Bu Me ether and phosphate buffer at 0° for 2 h while keeping pH at 7.0 by adding 0.5 N aqueous NaOH solution to give 43% (R)-1-(4-iodophenyl)ethanol (98% ee) and 44% (S)-1-(4-iodophenyl)ethyl chloroacetate (>98% ee) (VIII). VIII was coupled with Me 3H-imidazole-4-carboxylate using triphenylphosphine and di(tert-butyl) azocarboxylate in THF at -30° to 0° over 2.5 h to give 67% (R)-(+)-Me 3-[1-(4-iodophenyl)ethyl]-3H-imidazole-4-carboxylate (99% ee) which was refluxed with hexamethyltin in toluene at 135° for 17 h to give 96% (R)-(+)-Me 3-[1-[4-(trimethylstannyl)phenyl]ethyl]-3H-imidazole-4-carboxylate (IX). IX (30 µg) was reacted with [¹³¹I]iodide in 10-20 µL 0.05 N aqueous NaOH solution, 15 µL aqueous chloramine-T solution (1 mg/mL), and 6 µL 1 N aqueous HCl solution at room temperature for 1 min to give (R)-(+)-Me 3-[1-(4-[¹³¹I]iodophenyl)ethyl]-3H-imidazole-4-carboxylate (¹³¹I-MTO), i.e. II (R1 = R2 = Me, X = ¹³¹I).

IT **813466-09-0P**
 RL: BSU (Biological study, unclassified); DGN (Diagnostic use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of radiolabeled (phenylethyl)imidazolecarboxylic acid ester derivs. as positron-emission imaging agents for adrenal glands)

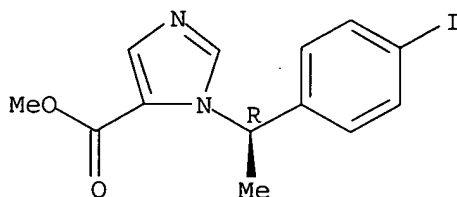
RN 813466-09-0 HCAPLUS
 CN 1H-Imidazole-5-carboxylic acid, 1-[(1R)-1-[4-(iodo-¹³¹I)phenyl]ethyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

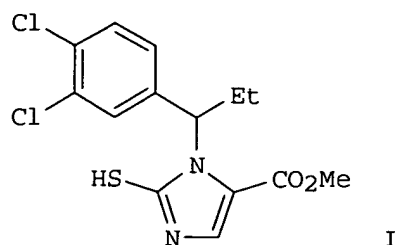


IT 813466-05-6P, (R)-(+)-Methyl 3-[1-(4-Iodophenyl)ethyl]-3H-imidazole-4-carboxylate
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of radiolabeled (phenylethyl)imidazolecarboxylic acid ester derivs. as positron-emission imaging agents for adrenal glands)
RN 813466-05-6 HCAPLUS
CN 1H-Imidazole-5-carboxylic acid, 1-[(1R)-1-(4-iodophenyl)ethyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



L4 ANSWER 2 OF 15 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2005:74646 HCAPLUS
DOCUMENT NUMBER: 142:280123
TITLE: 2-Mercaptoimidazoles, a new class of potent CCR2 antagonists
AUTHOR(S): Van Lommen, Guy; Doyon, Julien; Coesemans, Erwin; Boeckx, Staf; Cools, Marina; Buntinx, Mieke; Hermans, Bart; Van Wauwe, Jean
CORPORATE SOURCE: Inflammation Research, Johnson and Johnson Pharmaceutical Research and Development, Beerse, B-2340, Belg.
SOURCE: Bioorganic & Medicinal Chemistry Letters (2005), 15(3), 497-500
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

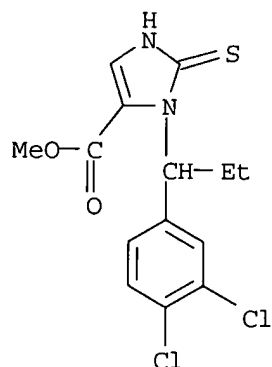


AB The synthesis and SAR of a class of CCR2 antagonists based on a 2-mercaptoimidazole scaffold, e.g., I. The initial lead compound was optimized to the corresponding optical active 3,4-disubstituted analogs, which have IC50 values in the MCP-1 induced Ca-flux below 0.01 μ M.

IT **112366-39-9P**
 RL: PAC (Pharmacological activity); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
 (preparation, CCR2 antagonistic activity, and structure-activity relationship of mercaptoimidazoles using heterocyclization as the key step)

RN 112366-39-9 HCAPLUS

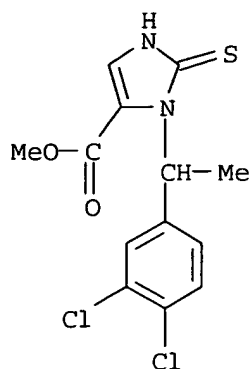
CN 1H-Imidazole-4-carboxylic acid, 3-[1-(3,4-dichlorophenyl)propyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)



IT **742107-74-0P 742107-75-1P 742107-79-5P**
742107-80-8P 742107-85-3P 742107-86-4P
742107-91-1P 742107-93-3P 742107-94-4P
742107-96-6P 742107-99-9P 742108-08-3P
742108-32-3P 742108-37-8P 847447-91-0P
847447-92-1P 847447-93-2P 847447-98-7P
847447-99-8P 847448-14-0P 847448-17-3P
 RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
 (preparation, CCR2 antagonistic activity, and structure-activity relationship of mercaptoimidazoles using heterocyclization as the key step)

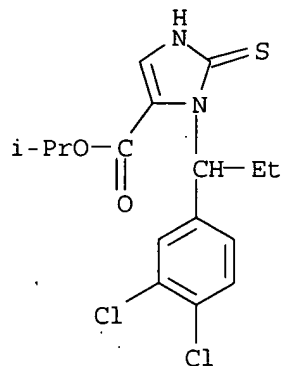
RN 742107-74-0 HCAPLUS

CN 1H-Imidazole-4-carboxylic acid, 3-[1-(3,4-dichlorophenyl)ethyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)



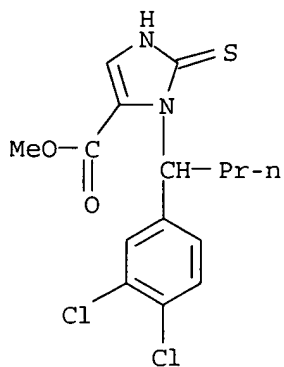
RN 742107-75-1 HCAPLUS

CN 1H-Imidazole-4-carboxylic acid, 3-[1-(3,4-dichlorophenyl)propyl]-2,3-dihydro-2-thioxo-, 1-methylethyl ester (9CI) (CA INDEX NAME)



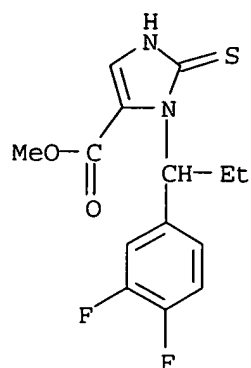
RN 742107-79-5 HCAPLUS

CN 1H-Imidazole-4-carboxylic acid, 3-[1-(3,4-dichlorophenyl)butyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)



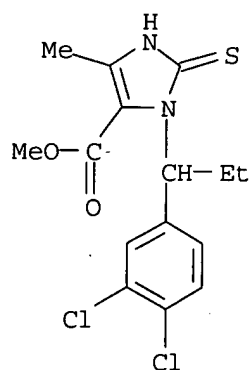
RN 742107-80-8 HCAPLUS

CN 1H-Imidazole-4-carboxylic acid, 3-[1-(3,4-difluorophenyl)propyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)



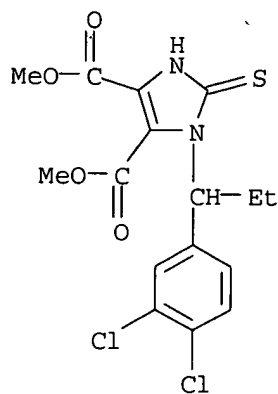
RN 742107-85-3 HCAPLUS

CN 1H-Imidazole-4-carboxylic acid, 3-[1-(3,4-dichlorophenyl)propyl]-2,3-dihydro-5-methyl-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)



RN 742107-86-4 HCAPLUS

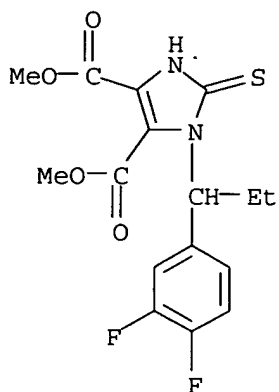
CN 1H-Imidazole-4,5-dicarboxylic acid, 1-[1-(3,4-dichlorophenyl)propyl]-2,3-dihydro-2-thioxo-, dimethyl ester (9CI) (CA INDEX NAME)



RN 742107-91-1 HCAPLUS

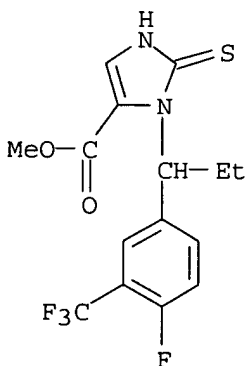
08/16/2005 10635294.trn

CN 1H-Imidazole-4,5-dicarboxylic acid, 1-[1-(3,4-difluorophenyl)propyl]-2,3-dihydro-2-thioxo-, dimethyl ester (9CI) (CA INDEX NAME)



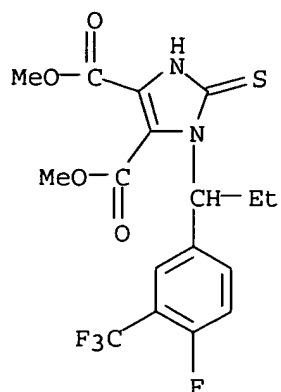
RN 742107-93-3 HCAPLUS

CN 1H-Imidazole-4-carboxylic acid, 3-[1-[4-fluoro-3-(trifluoromethyl)phenyl]propyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)



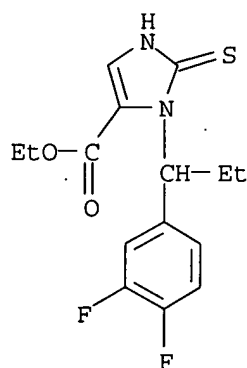
RN 742107-94-4 HCAPLUS

CN 1H-Imidazole-4,5-dicarboxylic acid, 1-[1-[4-fluoro-3-(trifluoromethyl)phenyl]propyl]-2,3-dihydro-2-thioxo-, dimethyl ester (9CI) (CA INDEX NAME)



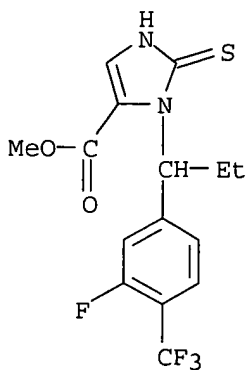
RN 742107-96-6 HCAPLUS

CN 1H-Imidazole-4-carboxylic acid, 3-[1-(3,4-difluorophenyl)propyl]-2,3-dihydro-2-thioxo-, ethyl ester (9CI) (CA INDEX NAME)



RN 742107-99-9 HCAPLUS

CN 1H-Imidazole-4-carboxylic acid, 3-[1-[3-fluoro-4-(trifluoromethyl)phenyl]propyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)

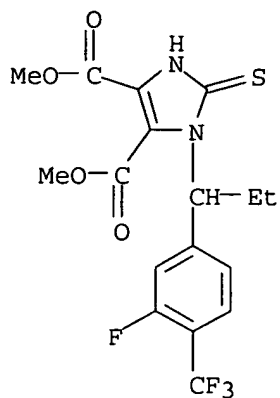


RN 742108-08-3 HCAPLUS

08/16/2005

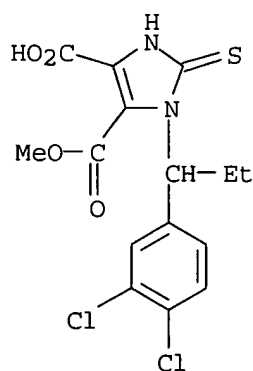
10635294.trn

CN 1H-Imidazole-4,5-dicarboxylic acid, 1-[1-[3-fluoro-4-(trifluoromethyl)phenyl]propyl]-2,3-dihydro-2-thioxo-, dimethyl ester (9CI) (CA INDEX NAME)



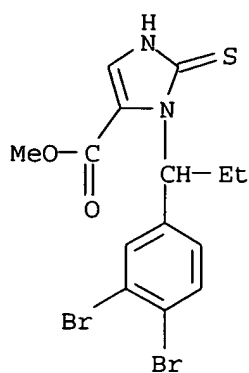
RN 742108-32-3 HCAPLUS

CN 1H-Imidazole-4,5-dicarboxylic acid, 1-[1-(3,4-dichlorophenyl)propyl]-2,3-dihydro-2-thioxo-, 5-methyl ester (9CI) (CA INDEX NAME)



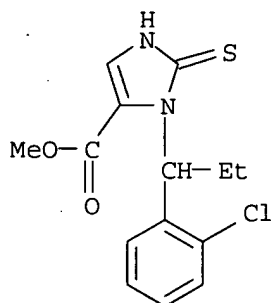
RN 742108-37-8 HCAPLUS

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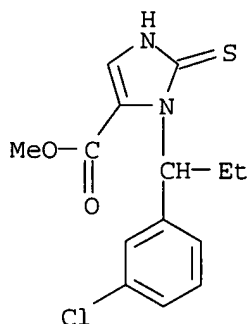
RN 847447-91-0 HCAPLUS

CN 1H-Imidazole-4-carboxylic acid, 3-[1-(2-chlorophenyl)propyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)



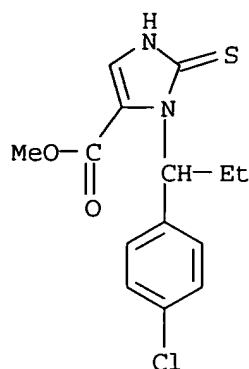
RN 847447-92-1 HCAPLUS

CN 1H-Imidazole-4-carboxylic acid, 3-[1-(3-chlorophenyl)propyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)



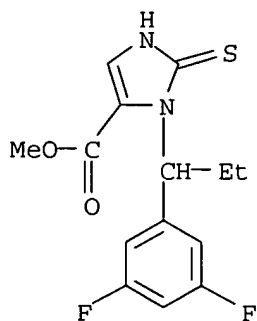
RN 847447-93-2 HCAPLUS

CN 1H-Imidazole-4-carboxylic acid, 3-[1-(4-chlorophenyl)propyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)



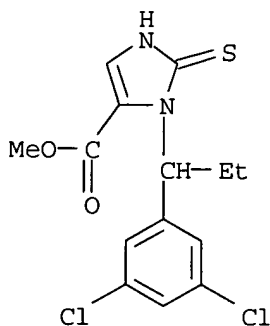
RN 847447-98-7 HCAPLUS

CN 1H-Imidazole-4-carboxylic acid, 3-[1-(3,5-difluorophenyl)propyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)



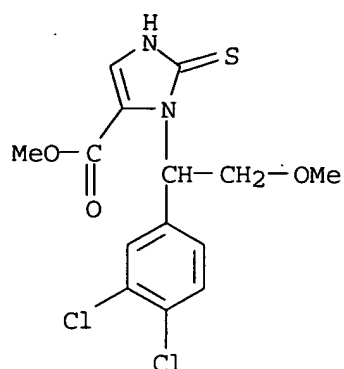
RN 847447-99-8 HCAPLUS

CN 1H-Imidazole-4-carboxylic acid, 3-[1-(3,5-dichlorophenyl)propyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)



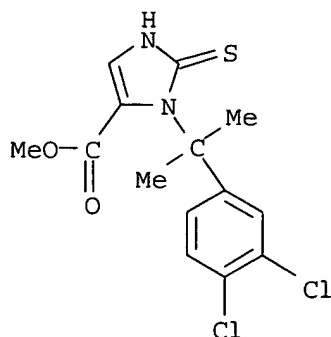
RN 847448-14-0 HCAPLUS

CN 1H-Imidazole-4-carboxylic acid, 3-[1-(3,4-dichlorophenyl)-2-methoxyethyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)



RN 847448-17-3 HCAPLUS

CN 1H-Imidazole-4-carboxylic acid, 3-[1-(3,4-dichlorophenyl)-1-methylethyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)



IT 742107-81-9P 742107-82-0P

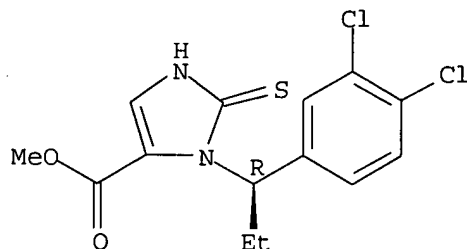
RL: PAC (Pharmacological activity); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)

(stereoselective preparation, CCR2 antagonistic activity, and structure-activity relationship of mercaptoimidazoles using asym. addition and heterocyclization as the key steps)

RN 742107-81-9 HCAPLUS

CN 1H-Imidazole-4-carboxylic acid, 3-[(1R)-1-(3,4-dichlorophenyl)propyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

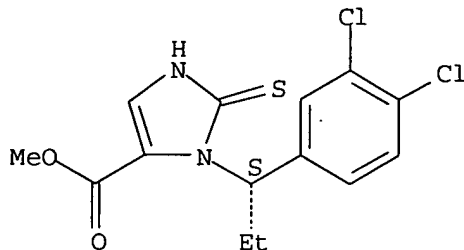


08/16/2005 10635294.trn

RN 742107-82-0 HCAPLUS

CN 1H-Imidazole-4-carboxylic acid, 3-[(1S)-1-(3,4-dichlorophenyl)propyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



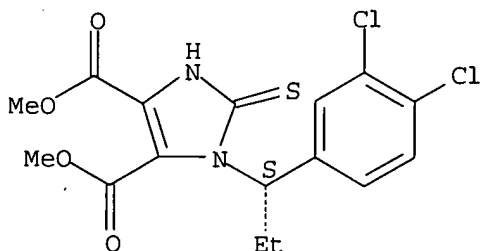
IT 847448-27-5P 847448-28-6P 847448-29-7P

RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(stereoselective preparation, CCR2 antagonistic activity, and structure-activity relationship of mercaptoimidazoles using asym. addition and heterocyclization as the key steps)

RN 847448-27-5 HCAPLUS

CN 1H-Imidazole-4,5-dicarboxylic acid, 1-[(1S)-1-(3,4-dichlorophenyl)propyl]-2,3-dihydro-2-thioxo-, dimethyl ester (9CI) (CA INDEX NAME)

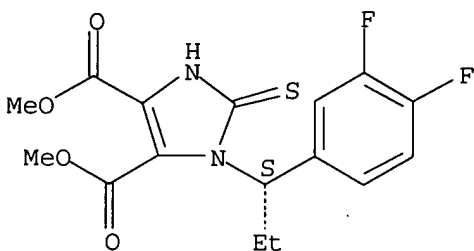
Absolute stereochemistry.



RN 847448-28-6 HCAPLUS

CN 1H-Imidazole-4,5-dicarboxylic acid, 1-[(1S)-1-(3,4-difluorophenyl)propyl]-2,3-dihydro-2-thioxo-, dimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

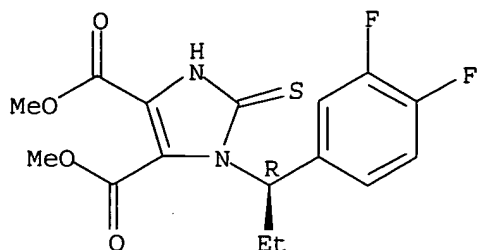


RN 847448-29-7 HCAPLUS

CN 1H-Imidazole-4,5-dicarboxylic acid, 1-[(1R)-1-(3,4-difluorophenyl)propyl]-

2,3-dihydro-2-thioxo-, dimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 15 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:686636 HCAPLUS

DOCUMENT NUMBER: 142:88850

TITLE: [123/131I]iodometomidate as a radioligand for functional diagnosis of adrenal disease: Synthesis, structural requirements and biodistribution

AUTHOR(S): Schirbel, A.; Zolle, I.; Hammerschmidt, F.; Berger, M. L.; Schiller, D.; Kvaternik, H.; Reiners, Chr.

CORPORATE SOURCE: Department of Nuclear Medicine, University of Wuerzburg, Germany

SOURCE: Radiochimica Acta (2004) 92(4-6), 297-303

CODEN: RAACAP; ISSN: 0033-8230

PUBLISHER: Oldenbourg Wissenschaftsverlag GmbH

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Metomidate [(R)-1-(1-phenylethyl)-1H-imidazole-5-carboxylic acid Me ester] (MTO, 1, Fig. 1) is a potent and selective inhibitor of the cytochrome P 450 enzyme system in the adrenal cortex. Labeled in the 4-position with radioiodine, (R)-4-[131I]iodometomidate, 2, [131I]IMTO has been evaluated by in-vitro studies and also ex-vivo in rats. [131I]IMTO was synthesized by oxidative radioiododestannylation using a suitable precursor which was prepared by a new stereoselective synthesis. Optimization of the labeling reaction was performed by systematic variation of the most important reaction parameters. Under optimum reaction conditions, a labeling yield of 95% was obtained. In-vitro-stability of the tracer was studied over 8 days, indicating slow deiodination (0.27%/h). Displacement studies using [131I]IMTO and rat adrenal membranes revealed the structural requirements for high affinity binding, namely an intact ester group and (R)-configuration of the radioligand. Pharmacokinetic studies in rats showed fast accumulation of [131I]IMTO in the adrenals (approx. 10% ID/g tissue) with an activity plateau for 2 h. Metabolic degradation was indicated by a steady increase of renal activity up to 4 h post injection. Based on target to non-target ratios the highest contrast for imaging of the adrenals was observed between 30 and 60 min post injection of [131I]IMTO. We conclude that SPECT using [123I]IMTO will be a promising method for the characterization of adrenal incidentalomas.

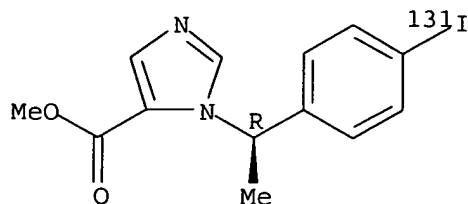
IT 813466-09-0

RL: BSU (Biological study, unclassified); BIOL (Biological study) (synthesis, structural requirements and biodistribution of [123/131I]iodometomidate as a radioligand for functional diagnosis of adrenal disease)

RN 813466-09-0 HCAPLUS

CN 1H-Imidazole-5-carboxylic acid, 1-[(1R)-1-[4-(iodo-131I)phenyl]ethyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



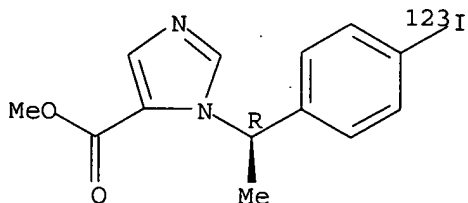
IT 813466-08-9P

RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis, structural requirements and biodistribution of [123/131I]iodometomidate as a radioligand for functional diagnosis of adrenal disease)

RN 813466-08-9 HCAPLUS

CN 1H-Imidazole-5-carboxylic acid, 1-[(1R)-1-[4-(iodo-123I)phenyl]ethyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



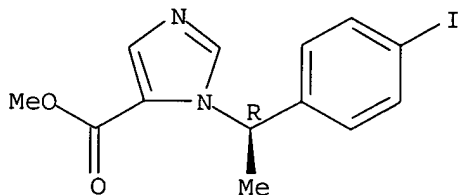
IT 813466-05-6P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis, structural requirements and biodistribution of [123/131I]iodometomidate as a radioligand for functional diagnosis of adrenal disease)

RN 813466-05-6 HCAPLUS

CN 1H-Imidazole-5-carboxylic acid, 1-[(1R)-1-(4-iodophenyl)ethyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



REFERENCE COUNT:

37

THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 15 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:675729 HCAPLUS

DOCUMENT NUMBER: 141:207206

TITLE: Preparation of mercaptoimidazoles as CCR2 receptor antagonists for the treatment of inflammatory disease

INVENTOR(S): Van Lommen, Guy Rosalia Eugeen; Doyon, Julien Georges Pierre-Olivier; Van Wauwe, Jean Pierre Frans; Cools, Marina Lucie Louise; Coesemans, Erwin

PATENT ASSIGNEE(S): Janssen Pharmaceutica N.V., Belg.

SOURCE: PCT Int. Appl., 64 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

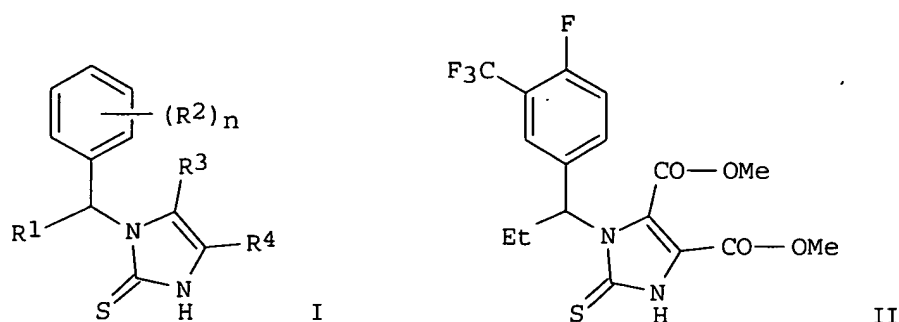
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004069809	A1	20040819	WO 2003-EP301038	20030203
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
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PRIORITY APPLN. INFO.: WO 2003-EP1038 A 20030203

OTHER SOURCE(S): MARPAT 141:207206

GI



AB The invention relates to mercaptoimidazoles of formula I, N-oxides, pharmaceutically acceptable addition salts, quaternary amines and stereochem. isomeric forms thereof, wherein R1 is H, (cyclo)alkyl, (hetero)aryl; R2 is halo, alkyl(oxy/thio), polyhaloalkyl(oxy), cyano, aminocarbonyl, (di)(alkyl)amino, nitro, aryl(oxy); R3 and R4 are H, cyano, (hydroxy)alkyl, C(O)OR5, C(O)NR6aR6b, S(O)2NR6aR6b, C(O)R7; R5 is a defined carbon or N-heterocyclic ester group; R6a, R6b is H, alkyl, (di)(alkyl)amino(alkyl), arylamino; or NR6aR6b is a N-heterocycle; R7 is H, alk(en/yn)yl, aryl, certain substituted alkyls; n is 1-5, etc., with some limitations. The compds. have been synthesized as CCR2 receptor antagonists and found useful for the treatment and prevention of diseases, such as inflammation, which are mediated through activation of the CCR2 receptor, particularly CCR2B receptor. The invention also relates to processes for preparing the compds. and pharmaceutical compns. comprising them. Thus, compound II was prepared from 1-[4-fluoro-3-(trifluoromethyl)phenyl]-1-propanone via oxime formation, reduction, N-alkylation with Me bromoacetate, formylation and finally cyclocondensation with (CO2Me)2 and KSCN. The synthesized compds. showed inhibition of MCP-1 induced Ca-flux in human THP-1 cells with pIC50 5.6-8.2 (pIC50 = -log IC50).

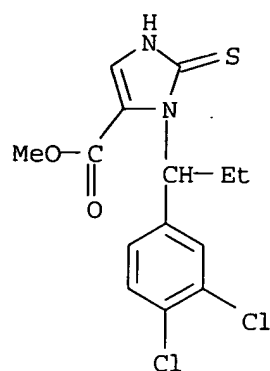
IT **112366-39-9P 742107-80-8P 742108-03-8P**

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(receptor antagonist; preparation of mercaptoimidazoles as CCR2 receptor antagonists for the treatment of inflammatory disease)

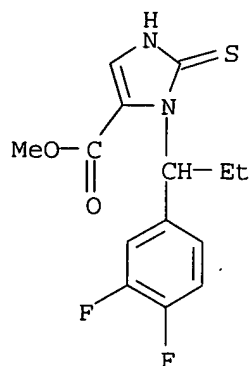
RN 112366-39-9 HCAPLUS

CN 1H-Imidazole-4-carboxylic acid, 3-[1-(3,4-dichlorophenyl)propyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)



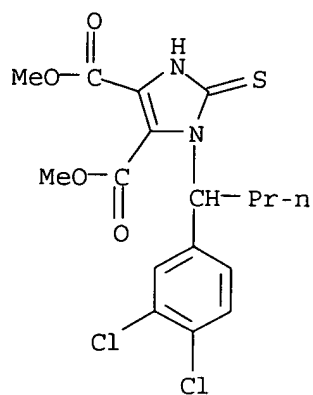
RN 742107-80-8 HCAPLUS

CN 1H-Imidazole-4-carboxylic acid, 3-[1-(3,4-difluorophenyl)propyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)



RN 742108-03-8 HCAPLUS

CN 1H-Imidazole-4,5-dicarboxylic acid, 1-[1-(3,4-dichlorophenyl)butyl]-2,3-dihydro-2-thioxo-, dimethyl ester (9CI) (CA INDEX NAME)

IT 91762-41-3P 92849-54-2P 112366-38-8P
112366-41-3P 742107-74-0P 742107-75-1P

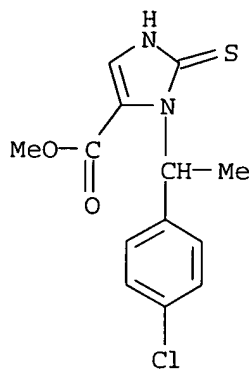
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742108-24-3P 742108-25-4P 742108-32-3P
742108-36-7P 742108-37-8P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
(Uses)

(receptor antagonist; preparation of mercaptoimidazoles as CCR2 receptor
antagonists for the treatment of inflammatory disease)

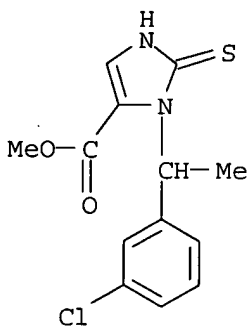
RN 91762-41-3 HCAPLUS

CN 1H-Imidazole-4-carboxylic acid, 3-[1-(4-chlorophenyl)ethyl]-2,3-dihydro-2-
thioxo-, methyl ester (9CI) (CA INDEX NAME)



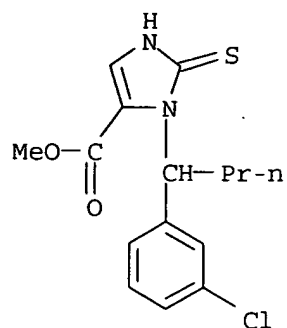
RN 92849-54-2 HCAPLUS

CN 1H-Imidazole-4-carboxylic acid, 3-[1-(3-chlorophenyl)ethyl]-2,3-dihydro-2-
thioxo-, methyl ester (9CI) (CA INDEX NAME)



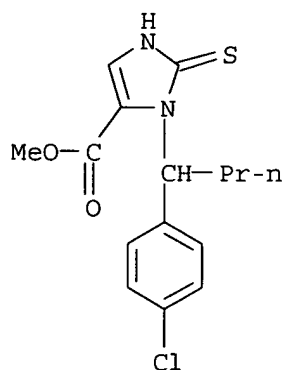
RN 112366-38-8 HCAPLUS

CN 1H-Imidazole-4-carboxylic acid, 3-[1-(3-chlorophenyl)butyl]-2,3-dihydro-2-
thioxo-, methyl ester (9CI) (CA INDEX NAME)



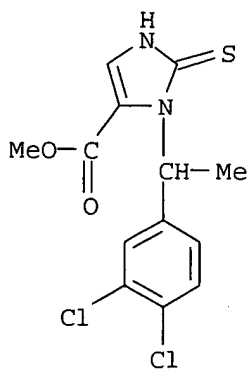
RN 112366-41-3 HCAPLUS

CN 1H-Imidazole-4-carboxylic acid, 3-[1-(4-chlorophenyl)butyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)



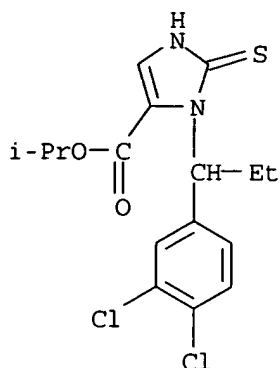
RN 742107-74-0 HCAPLUS

CN 1H-Imidazole-4-carboxylic acid, 3-[1-(3,4-dichlorophenyl)ethyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)

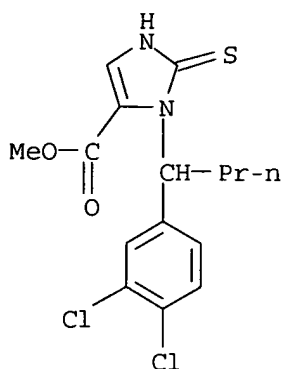


RN 742107-75-1 HCAPLUS

CN 1H-Imidazole-4-carboxylic acid, 3-[1-(3,4-dichlorophenyl)propyl]-2,3-dihydro-2-thioxo-, 1-methylethyl ester (9CI) (CA INDEX NAME)

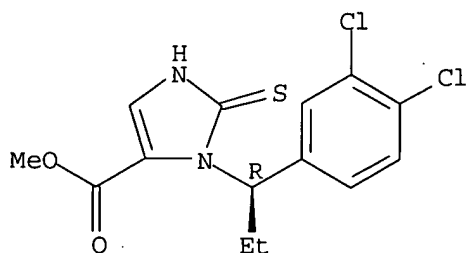


RN 742107-79-5 HCAPLUS
CN 1H-Imidazole-4-carboxylic acid, 3-[1-(3,4-dichlorophenyl)butyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)



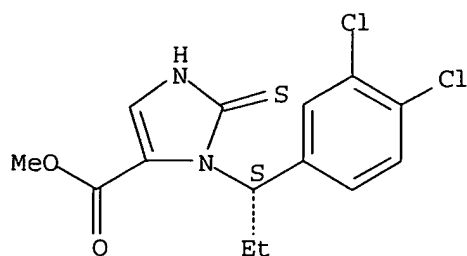
RN 742107-81-9 HCAPLUS
CN 1H-Imidazole-4-carboxylic acid, 3-[(1R)-1-(3,4-dichlorophenyl)propyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



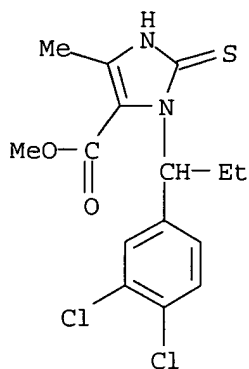
RN 742107-82-0 HCAPLUS
CN 1H-Imidazole-4-carboxylic acid, 3-[(1S)-1-(3,4-dichlorophenyl)propyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



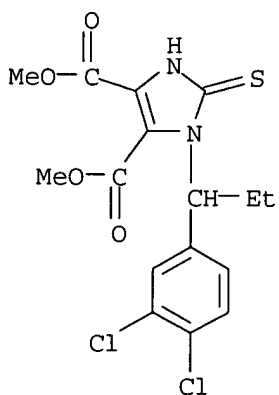
RN 742107-85-3 HCAPLUS

CN 1H-Imidazole-4-carboxylic acid, 3-[1-(3,4-dichlorophenyl)propyl]-2,3-dihydro-5-methyl-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)



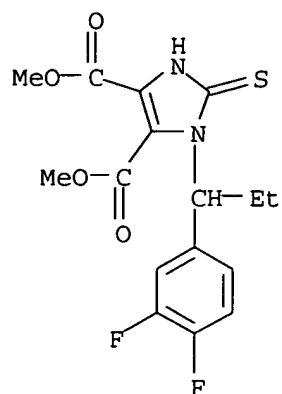
RN 742107-86-4 HCAPLUS

CN 1H-Imidazole-4,5-dicarboxylic acid, 1-[1-(3,4-dichlorophenyl)propyl]-2,3-dihydro-2-thioxo-, dimethyl ester (9CI) (CA INDEX NAME)



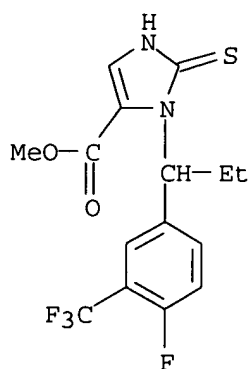
RN 742107-91-1 HCAPLUS

CN 1H-Imidazole-4,5-dicarboxylic acid, 1-[1-(3,4-difluorophenyl)propyl]-2,3-dihydro-2-thioxo-, dimethyl ester (9CI) (CA INDEX NAME)



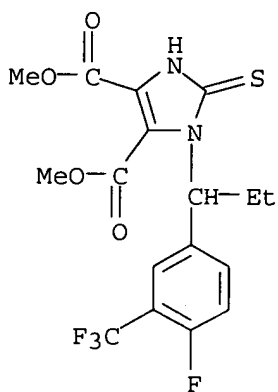
RN 742107-93-3 HCAPLUS

CN 1H-Imidazole-4-carboxylic acid, 3-[1-[4-fluoro-3-(trifluoromethyl)phenyl]propyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI)
(CA INDEX NAME)



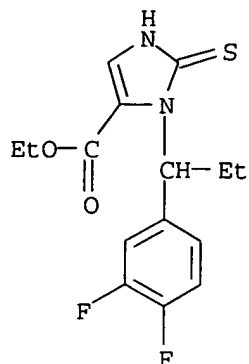
RN 742107-94-4 HCAPLUS

CN 1H-Imidazole-4,5-dicarboxylic acid, 1-[1-[4-fluoro-3-(trifluoromethyl)phenyl]propyl]-2,3-dihydro-2-thioxo-, dimethyl ester
(9CI) (CA INDEX NAME)



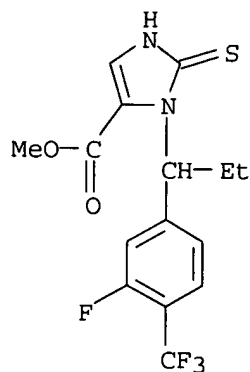
RN 742107-96-6 HCAPLUS

CN 1H-Imidazole-4-carboxylic acid, 3-[1-(3,4-difluorophenyl)propyl]-2,3-dihydro-2-thioxo-, ethyl ester (9CI) (CA INDEX NAME)



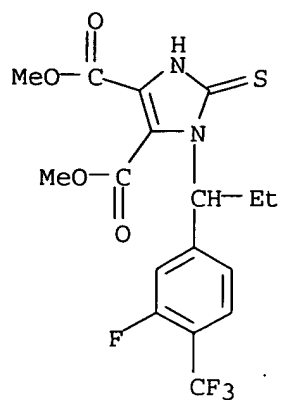
RN 742107-99-9 HCAPLUS

CN 1H-Imidazole-4-carboxylic acid, 3-[1-[3-fluoro-4-(trifluoromethyl)phenyl]propyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)



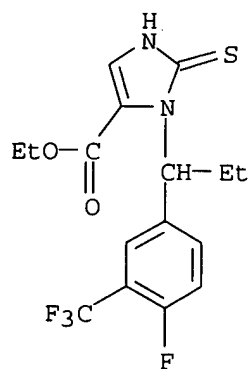
RN 742108-08-3 HCAPLUS

CN 1H-Imidazole-4,5-dicarboxylic acid, 1-[1-[3-fluoro-4-(trifluoromethyl)phenyl]propyl]-2,3-dihydro-2-thioxo-, dimethyl ester (9CI) (CA INDEX NAME)



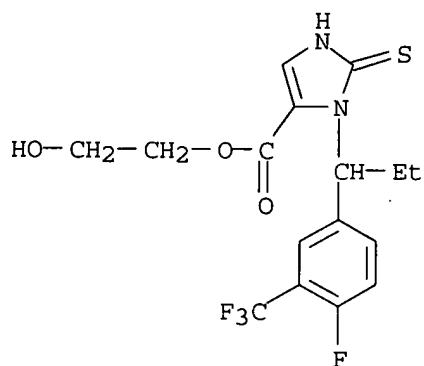
RN 742108-09-4 HCAPLUS

CN 1H-Imidazole-4-carboxylic acid, 3-[1-[4-fluoro-3-(trifluoromethyl)phenyl]propyl]-2,3-dihydro-2-thioxo-, ethyl ester (9CI)
(CA INDEX NAME)



RN 742108-10-7 HCAPLUS

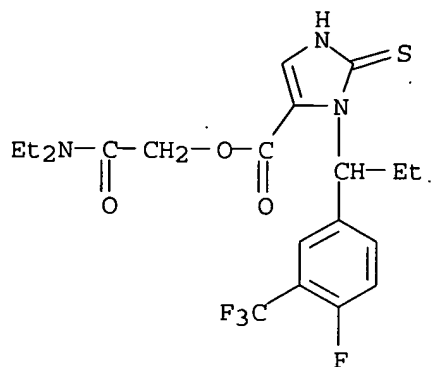
CN 1H-Imidazole-4-carboxylic acid, 3-[1-[4-fluoro-3-(trifluoromethyl)phenyl]propyl]-2,3-dihydro-2-thioxo-, 2-hydroxyethyl ester (9CI) (CA INDEX NAME)



08/16/2005 10635294.trn

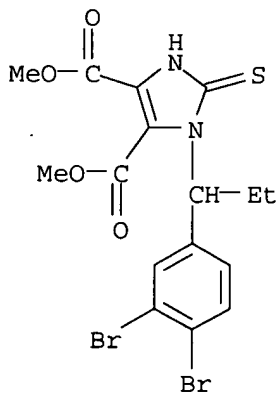
RN 742108-13-0 HCAPLUS

CN 1H-Imidazole-4-carboxylic acid, 3-[1-[4-fluoro-3-(trifluoromethyl)phenyl]propyl]-2,3-dihydro-2-thioxo-, 2-(diethylamino)-2-oxoethyl ester (9CI) (CA INDEX NAME)



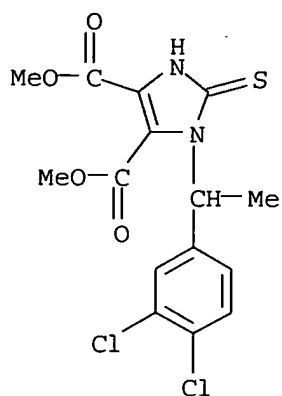
RN 742108-18-5 HCAPLUS

CN 1H-Imidazole-4,5-dicarboxylic acid, 1-[1-(3,4-dibromophenyl)propyl]-2,3-dihydro-2-thioxo-, dimethyl ester (9CI) (CA INDEX NAME)



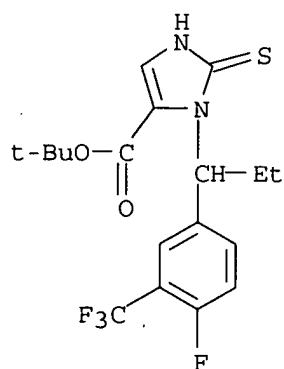
RN 742108-24-3 HCAPLUS

CN 1H-Imidazole-4,5-dicarboxylic acid, 1-[1-(3,4-dichlorophenyl)ethyl]-2,3-dihydro-2-thioxo-, dimethyl ester (9CI) (CA INDEX NAME)



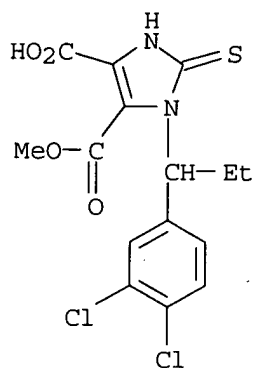
RN 742108-25-4 HCAPLUS

CN 1H-Imidazole-4-carboxylic acid, 3-[1-[4-fluoro-3-(trifluoromethyl)phenyl]propyl]-2,3-dihydro-2-thioxo-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



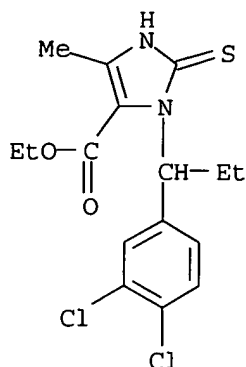
RN 742108-32-3 HCAPLUS

CN 1H-Imidazole-4,5-dicarboxylic acid, 1-[1-(3,4-dichlorophenyl)propyl]-2,3-dihydro-2-thioxo-, 5-methyl ester (9CI) (CA INDEX NAME)



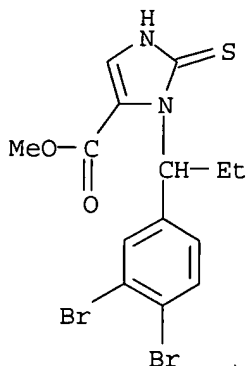
RN 742108-36-7 HCAPLUS

CN 1H-Imidazole-4-carboxylic acid, 3-[1-(3,4-dichlorophenyl)propyl]-2,3-dihydro-5-methyl-2-thioxo-, ethyl ester (9CI) (CA INDEX NAME)



RN 742108-37-8 HCAPLUS

CN 1H-Imidazole-4-carboxylic acid, 3-[1-(3,4-dibromophenyl)propyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)



L4 ANSWER 5 OF 15 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1989:69236 HCAPLUS

DOCUMENT NUMBER: 110:69236

TITLE: Comparative effects of etomidate and its fluoro analog, R 8110, on testicular, adrenal and ovarian steroid biosynthesis

AUTHOR(S): De Coster, R.; Wouters, W.; Beerens, D.; Haelterman, C.; Doolaeghe, R.; Goeminne, N.; Krekels, M.

CORPORATE SOURCE: Dep. Endocrinol. Oncol., Janssen Res. Found., Beerse, B-2340, Belg.

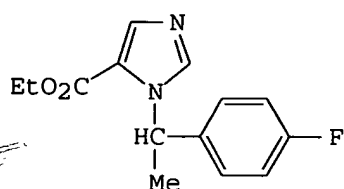
SOURCE: Journal of Veterinary Pharmacology and Therapeutics (1988), 11(4), 345-53

CODEN: JVPTD9; ISSN: 0140-7783

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



AB The effects of etomidate and its fluoro analog R 8110 (I) on adrenal, testicular, and ovarian steroid biosynthesis were compared in cultures of guinea pig adrenal, rat adrenal capsular, rat testicular, and rat ovarian granulosa cells. At 100 nM, etomidate inhibited the adrenal 11-hydroxylation of glucocorticoid and mineralocorticoid biosyntheses, causing a decrease in cortisol and corticosterone and an accumulation of 11-deoxycortisol and 11-deoxycorticosterone in guinea pig adrenal and rat capsular adrenal cell suspensions, resp. At higher concns. (>10⁻⁶M), etomidate also inhibited ovarian estradiol production, testicular androgen formation, and ovarian progesterone synthesis. The latter action suggests an effect on ovarian aromatase, on testicular 17 α /17,20-lyase activities, and on cholesterol side-chain cleavage. The fluoro analog R 8110 was 10-times less potent as an inhibitor of 11-hydroxylation and slightly affected progesterone formation only in adrenal cell suspensions. Testosterone production was less affected by R 8110 than by etomidate. The increase of progestins suggests that the 17 α /17,20-lyase activities are the most sensitive testicular enzymic reactions to R 8110. For inhibition of ovarian estradiol production, R 8110 was 20-times more potent than etomidate.

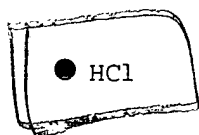
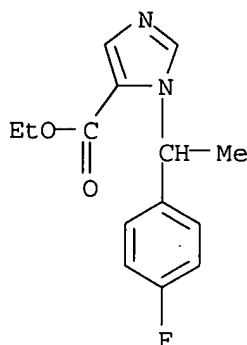
IT 109872-40-4, R 8110

RL: BIOL (Biological study)

(steroidogenesis by adrenal and ovarian and testicular cells response to)

RN 109872-40-4 HCAPLUS

CN 1H-Imidazole-5-carboxylic acid, 1-[1-(4-fluorophenyl)ethyl]-, ethyl ester, monohydrochloride (9CI) (CA INDEX NAME)



ACCESSION NUMBER: 1988:400609 HCAPLUS
 DOCUMENT NUMBER: 109:609
 TITLE: Hypnoanalgesia with R 8110/fentanyl in the dog: pharmacodynamic and pharmacokinetic interactions
 AUTHOR(S): Monbaliu, J.; Degryse, A. D.; Ooms, L. A. A.; Van Dijk, P.; Lagerweij, E.; Michiels, M.; Woestenborghs, R.; Heykants, J.
 CORPORATE SOURCE: Dep. Drug Metab. Pharmacokinet., Janssen Pharm., Beerse, B-2340, Belg.
 SOURCE: Journal of Veterinary Pharmacology and Therapeutics (1988), 11(1), 63-70
~~CODEN: JVPSTD9~~; ISSN: 0140-7783

DOCUMENT TYPE: Journal
 LANGUAGE: English

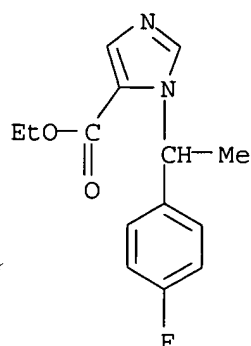
AB The pharmacokinetics and clin. effects of the short-acting hypnotic R 8110 and of the narcotic analgesic fentanyl were studied in the dog. The effects of sep. i.v. injections of R 8110 (4 mg/kg) and fentanyl (0.015 mg/kg) and of concurrent i.v. injection of the 2 were studied. After administration of R 8110, induction of hypnosis occurred within 1 min, maximal depth of anesthesia and satisfactory analgesia and muscle relaxation were obtained after 5 min. The effects had decreased within 15 min and full recovery occurred within 30 min. Fentanyl alone produced neither hypnosis nor muscle relaxation. When fentanyl and R 8110 were given simultaneously, the duration of hypnosis was doubled in comparison with R 8110 alone. Moreover, markedly improved and longer lasting analgesia and muscle relaxation were observed with the combination. When the drugs were injected together, the plasma concns. of R 8110 were initially much higher than after sep. injection of R 8110, but they became similar after 30 min. Although statistically non-significant, fentanyl reduced the total plasma clearance of R 8110 and decreased the volume of distribution. Fentanyl did not alter the elimination half-life of R 8110. R 8110 had no apparent influence on the pharmacokinetics of fentanyl.

IT 109872-40-4, R 8110 114705-71-4

RL: BIOL (Biological study)
 (hypnoanalgesia with, in dogs, pharmacokinetics in relation to)

RN 109872-40-4 HCAPLUS

CN 1H-Imidazole-5-carboxylic acid, 1-[1-(4-fluorophenyl)ethyl]-, ethyl ester, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 114705-71-4 HCAPLUS

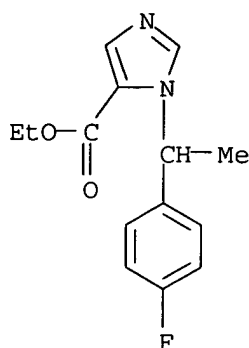
08/16/2005 10635294.trn

CN 1H-Imidazole-5-carboxylic acid, 1-[1-(4-fluorophenyl)ethyl]-, ethyl ester, monohydrochloride, mixt. with N-phenyl-N-[1-(2-phenylethyl)-4-piperidinyl]propanamide (9CI) (CA INDEX NAME)

CM 1

CRN 109872-40-4

CMF C14 H15 F N2 O2 . Cl H

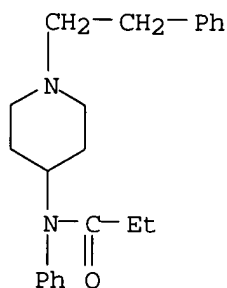


● HCl

CM 2

CRN 437-38-7

CMF C22 H28 N2 O



L4 ANSWER 7 OF 15 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1988:167377 HCAPLUS

DOCUMENT NUMBER: 108:167377

TITLE: Synthesis of (R)-(+)-3H-etomidate

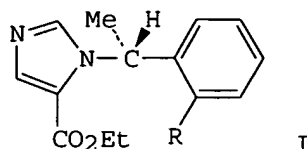
AUTHOR(S): Janssen, Cor G. M.; Thijssen, Jos B. A.; Verluyten, Willy L. M.; Heykants, Jozef J. P.

CORPORATE SOURCE: Dep. Drug Metab. Pharmacokinet., Janssen Pharm., Beerse, B-2340, Belg.

SOURCE: Journal of Labelled Compounds and Radiopharmaceuticals (1987), 24(8), 909-18

CODEN: JLCRD4; ISSN: 0362-4803

DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 108:167377
 GI



AB Etomidate, (R)-(+)-ethyl-1-(1-phenylethyl)-1H-imidazole-5-carboxylate (I, R = H) is a short-acting hypnotic. A new synthesis, featuring optical resolution on a non-radioactive precursor and introduction of the tritium label by reductive dehalogenation of I (R = Br) is described. I (R = T) was obtained at a specific activity of 3.77 Ci/mmol and a 99.9% purity.

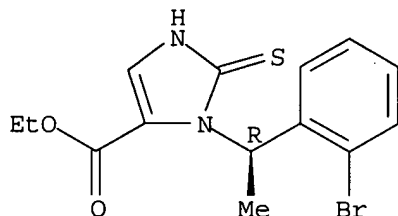
IT 112366-36-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and desulfurization of, with sodium nitrite)

RN 112366-36-6 HCAPLUS

CN 1H-Imidazole-4-carboxylic acid, 3-[1-(2-bromophenyl)ethyl]-2,3-dihydro-2-thioxo-, ethyl ester, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 112366-50-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 112366-50-4 HCAPLUS

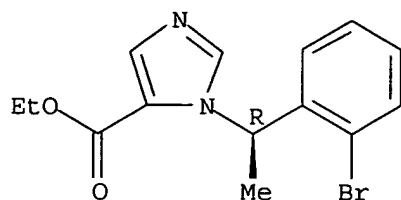
CN 1H-Imidazole-5-carboxylic acid, 1-[1-(2-bromophenyl)ethyl]-, ethyl ester, (R)-, sulfate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 112366-49-1

CMF C14 H15 Br N2 O2

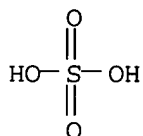
Absolute stereochemistry.



CM 2

CRN 7664-93-9

CMF H2 O4 S



IT 112366-49-1P

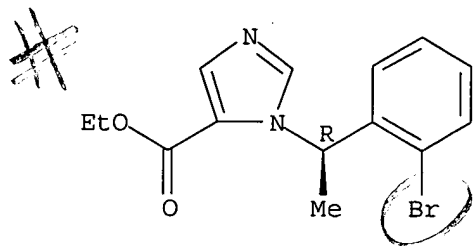
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation, reductive debromination, and tritiation of)

RN 112366-49-1 HCAPLUS

CN 1H-Imidazole-5-carboxylic acid, 1-[1-(2-bromophenyl)ethyl]-, ethyl ester, (R) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 8 OF 15 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1988:112460 HCAPLUS

DOCUMENT NUMBER: 108:112460

TITLE: Preparation of arylalkylimidazoles as antiepileptics

INVENTOR(S): Allgeier, Hans

PATENT ASSIGNEE(S): Ciba-Geigy A.-G. , Switz.

SOURCE: Eur. Pat. Appl., 40 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

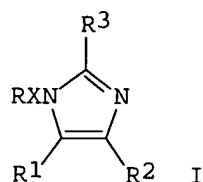
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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EP 248414 A2 19871209 EP 1987-108017 19870603
 EP 248414 A3 19880127
 EP 248414 B1 19920923
 R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE
 US 4851424 A 19890725 US 1987-53913 19870526
~~US 82726~~ A1 19911215 IL 1987-82726 19870601
 EL 8702489 A 19871207 FI 1987-2489 19870603
 AT 80876 E 19921015 AT 1987-108017 19870603
 DK 8702892 A 19871207 DK 1987-2892 19870604
 DD 260928 A5 19881012 DD 1987-303543 19870604
 NO 8702393 A 19871207 NO 1987-2393 19870605
 NO 168103 B 19911007
 NO 168103 C 19920115
 AU 8773896 A1 19871210 AU 1987-73896 19870605
 AU 610501 B2 19910523
 JP 62292763 A2 19871219 JP 1987-140124 19870605
 ZA 8704042 A 19880224 ZA 1987-4042 19870605
 HU 45509 A2 19880728 HU 1987-2588 19870605
 HU 207050 B 19930301

PRIORITY APPLN. INFO.:

CH 1986-2294 A 19860606
 CH 1986-4034 A 19861009
 EP 1987-108017 A 19870603

GI



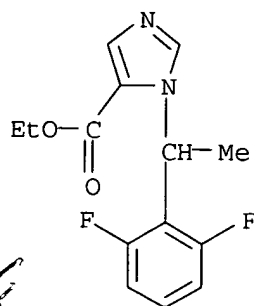
AB The title compds. [I; R = alkyl- or halo-substituted Ph; R1, R2 = (substituted) carbamoyl, H, alkyl; R3 = H, alkyl; X = alkylene] were prepared as antiepileptics. 2,6-Difluorobenzylamine and 2-isocyano-3-dimethylaminoacrylic acid were refluxed 3 h in PhMe to give 1-(2,6-difluorobenzyl)imidazole-4-(N,N-dimethyl)carboxamide.

IT 113212-12-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of, as antiepileptic intermediate)

RN 113212-12-7 HCAPLUS

CN 1H-Imidazole-5-carboxylic acid, 1-[1-(2,6-difluorophenyl)ethyl]-, ethyl ester (9CI) (CA INDEX NAME)



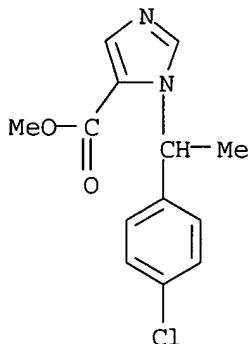
which are new, are useful as herbicides. NaOMe in THF was treated with HCO₂Me and Me N-formyl-N-[1-(4-methylphenyl)butyl]glycine, to give I (R₁ = SH, R₂ = Me, Z = 4-MeC₆H₄, A = Pr). Pre-emergence I [R₁ = H, R₂ = Me, Z = Z = 2-(MeO)C₆H₄, A = Pr (1 kg/ha) controlled, *Digitaria sanguinalis*, *Galium aparine* and other weeds with no toxicity to corn. Dust formulations were made of I 2, SiO₂, 1, and talc 97%.

IT 2852-45-1P 2852-47-3P 2852-49-5P
 2852-51-9P 2881-39-2P 84946-23-6P
 91761-91-0P 91762-40-2P 91762-41-3P
 92027-89-9P 92849-54-2P 109872-40-4P
 112365-99-8P 112366-35-5P 112366-36-6P
 112366-38-8P 112366-39-9P 112366-40-2P
 112366-41-3P 112366-42-4P 112366-43-5P
 112366-50-4P 112366-53-7P 112366-55-9P
 112366-56-0P 112366-57-1P 112366-60-6P
 112366-82-2P 112367-07-4P 112367-08-5P
 112367-12-1P 112367-28-9P 112367-29-0P
 112367-32-5P 112367-33-6P 112367-34-7P
 112367-37-0P 112367-47-2P 112421-35-9P
 112421-37-1P

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of, as herbicide)

RN 2852-45-1 HCAPLUS

CN 1H-Imidazole-5-carboxylic acid, 1-[1-(4-chlorophenyl)ethyl]-, methyl ester, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 2852-47-3 HCAPLUS

CN 1H-Imidazole-5-carboxylic acid, 1-[1-(3-chlorophenyl)ethyl]-, methyl ester, monohydrochloride (9CI) (CA INDEX NAME)

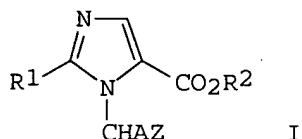
L4 ANSWER 9 OF 15 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1988:51267 HCAPLUS
 DOCUMENT NUMBER: 108:51267
 TITLE: Imidazolecarboxylate herbicides
 INVENTOR(S): Van Gestel, Jozef Frans Elisabe; Lutz, William R.; Van Lommen, Guy Rosalia Eugene; Fischer, Hanspeter; Schroyen, Marc Francis Josephin; Thummel, Rudolph C.
 PATENT ASSIGNEE(S): Janssen Pharmaceutica N. V., Belg.
 SOURCE: Eur. Pat. Appl., 42 pp.
 CODEN: EPXXDW
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

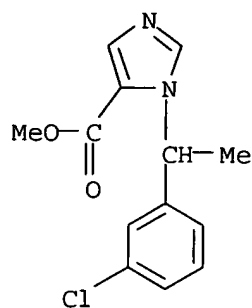
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 240050	A1	19871007	EP 1987-200390	19870304
EP 240050	B1	19910626		
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
US 4770689	A	19880913	US 1986-944694	19861219
SU 1558302	A3	19900415	SU 1987-4202079	19870303
AT 64678	E	19910715	AT 1987-200390	19870304
PL 149675	B1	19900331	PL 1987-264461	19870305
DK 8701214	A	19870911	DK 1987-1214	19870309
AU 8769831	A1	19870917	AU 1987-69831	19870309
AU 597038	B2	19900524		
ZA 8701693	A	19881026	ZA 1987-1693	19870309
IL 81831	A1	19910512	IL 1987-81831	19870309
CA 1289142	A1	19910917	CA 1987-531464	19870309
CN 87101880	A	19870923	CN 1987-101880	19870310
CN 1023317	B	19931229		
JP 62277363	A2	19871202	JP 1987-53190	19870310
BR 8701097	A	19871229	BR 1987-1097	19870310
HU 44405	A2	19880328	HU 1987-1005	19870310
HU 201451	B	19901128		

PRIORITY APPLN. INFO.:
 US 1986-838067 A 19860310
 US 1986-944694 A 19861219
 EP 1987-200390 A 19870304

OTHER SOURCE(S): CASREACT 108:51267
 GI



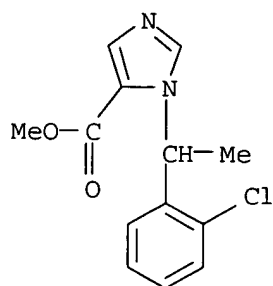
AB The imidazolecarboxylates I [R1 = H, SH; R2 = H, alkyl, alkynyl, alkyloxyalkyl, aryl alkyl, (un)substituted Ph, etc., A = H, cycloalkyl, alkylcycloalkyl, alkyl, (un)substituted pyridinyl, pyrimidinyl, furanyl, thienyl, etc.; Z = (un)substituted thienyl, Ph, pyridinyl, etc.] some of



● HCl

RN 2852-49-5 HCAPLUS

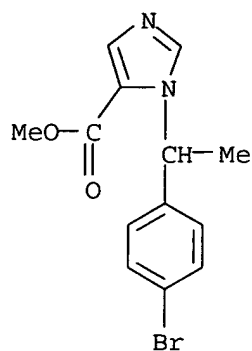
CN 1H-Imidazole-5-carboxylic acid, 1-[1-(2-chlorophenyl)ethyl]-, methyl ester, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 2852-51-9 HCAPLUS

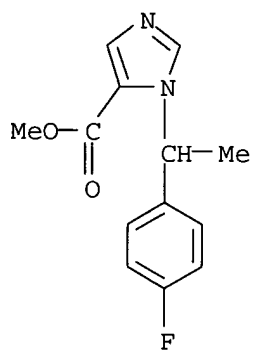
CN 1H-Imidazole-5-carboxylic acid, 1-[1-(4-bromophenyl)ethyl]-, methyl ester, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 2881-39-2 HCAPLUS

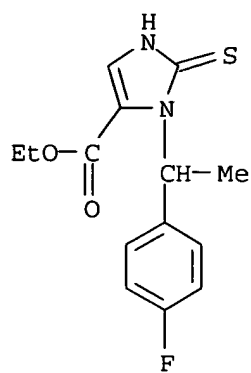
CN 1H-Imidazole-5-carboxylic acid, 1-[1-(4-fluorophenyl)ethyl]-, methyl ester, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

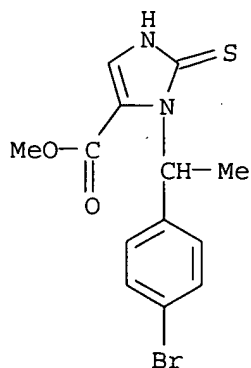
RN 84946-23-6 HCAPLUS

CN 1H-Imidazole-4-carboxylic acid, 3-[1-(4-fluorophenyl)ethyl]-2,3-dihydro-2-thioxo-, ethyl ester (9CI) (CA INDEX NAME)



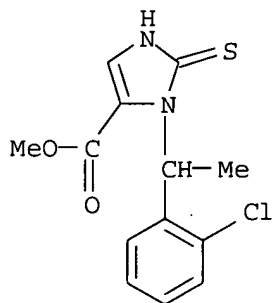
RN 91761-91-0 HCAPLUS

CN 1H-Imidazole-4-carboxylic acid, 3-[1-(4-bromophenyl)ethyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)



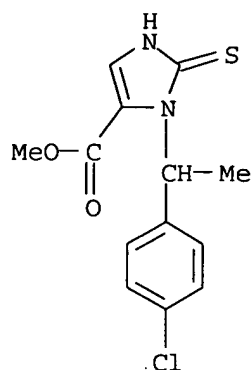
RN 91762-40-2 HCAPLUS

CN 1H-Imidazole-4-carboxylic acid, 3-[1-(2-chlorophenyl)ethyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)



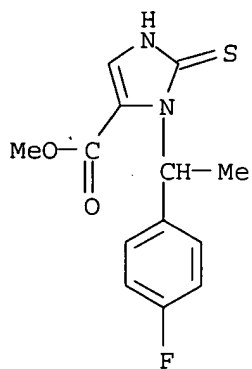
RN 91762-41-3 HCAPLUS

CN 1H-Imidazole-4-carboxylic acid, 3-[1-(4-chlorophenyl)ethyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)



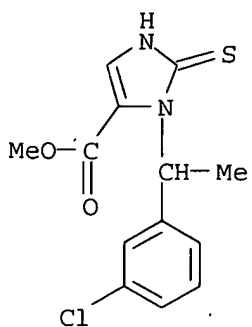
RN 92027-89-9 HCAPLUS

CN 1H-Imidazole-4-carboxylic acid, 3-[1-(4-fluorophenyl)ethyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)



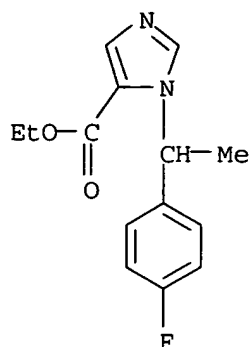
RN 92849-54-2 HCAPLUS

CN 1H-Imidazole-4-carboxylic acid, 3-[1-(3-chlorophenyl)ethyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)



RN 109872-40-4 HCAPLUS

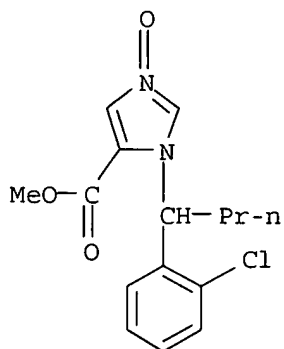
CN 1H-Imidazole-5-carboxylic acid, 1-[1-(4-fluorophenyl)ethyl]-, ethyl ester, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

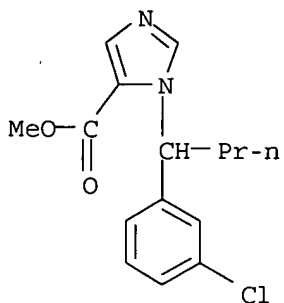
RN 112365-99-8 HCAPLUS

CN 1H-Imidazole-5-carboxylic acid, 1-[1-(2-chlorophenyl)butyl]-, methyl ester, 3-oxide (9CI) (CA INDEX NAME)



RN 112366-35-5 HCAPLUS

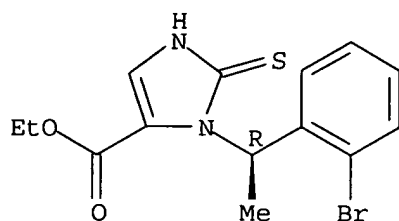
CN 1H-Imidazole-5-carboxylic acid, 1-[1-(3-chlorophenyl)butyl]-, methyl ester (9CI) (CA INDEX NAME)



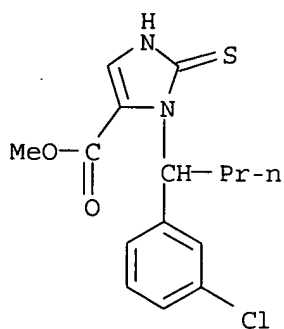
RN 112366-36-6 HCAPLUS

CN 1H-Imidazole-4-carboxylic acid, 3-[1-(2-bromophenyl)ethyl]-2,3-dihydro-2-thioxo-, ethyl ester, (R)- (9CI) (CA INDEX NAME)

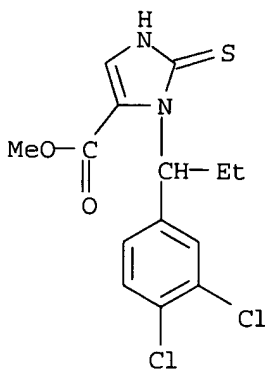
Absolute stereochemistry.



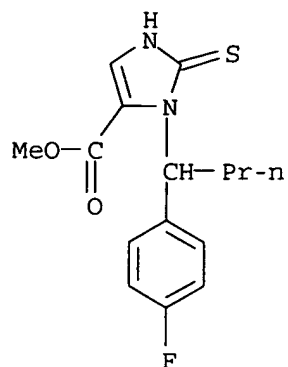
RN 112366-38-8 HCAPLUS
CN 1H-Imidazole-4-carboxylic acid, 3-[1-(3-chlorophenyl)butyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)



RN 112366-39-9 HCAPLUS
CN 1H-Imidazole-4-carboxylic acid, 3-[1-(3,4-dichlorophenyl)propyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)

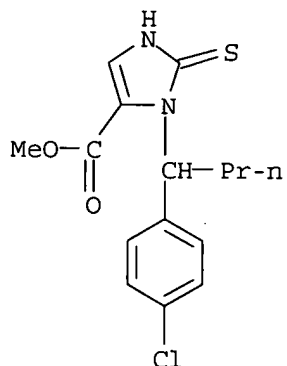


RN 112366-40-2 HCAPLUS
CN 1H-Imidazole-4-carboxylic acid, 3-[1-(4-fluorophenyl)butyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)



RN 112366-41-3 HCAPLUS

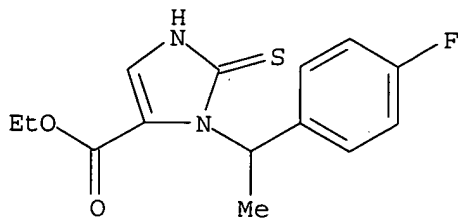
CN 1H-Imidazole-4-carboxylic acid, 3-[1-(4-chlorophenyl)butyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)



RN 112366-42-4 HCAPLUS

CN 1H-Imidazole-4-carboxylic acid, 3-[1-(4-fluorophenyl)ethyl]-2,3-dihydro-2-thioxo-, ethyl ester, (-)-(9CI) (CA INDEX NAME)

Rotation (-).



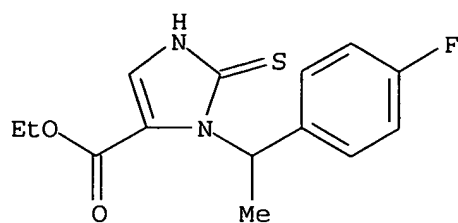
RN 112366-43-5 HCAPLUS

CN 1H-Imidazole-4-carboxylic acid, 3-[1-(4-fluorophenyl)ethyl]-2,3-dihydro-2-thioxo-, ethyl ester, (+)-(9CI) (CA INDEX NAME)

Rotation (+).

08/16/2005

10635294.trn



RN 112366-50-4 HCAPLUS

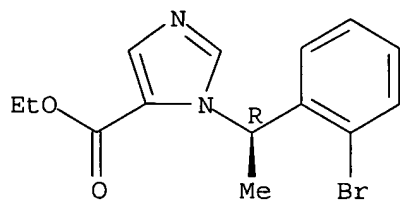
CN 1H-Imidazole-5-carboxylic acid, 1-[1-(2-bromophenyl)ethyl]-, ethyl ester, (R)-, sulfate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 112366-49-1

CMF C14 H15 Br N2 O2

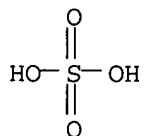
Absolute stereochemistry.



CM 2

CRN 7664-93-9

CMF H2 O4 S



RN 112366-53-7 HCAPLUS

CN 1H-Imidazole-5-carboxylic acid, 1-[1-(2,5-dichlorophenyl)butyl]-, methyl ester, mononitrate (9CI) (CA INDEX NAME)

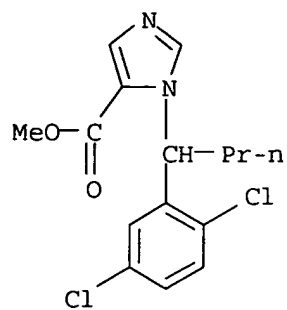
CM 1

CRN 112366-52-6

CMF C15 H16 Cl2 N2 O2

08/16/2005

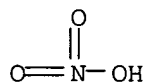
10635294.trn



CM 2

CRN 7697-37-2

CMF H N O3



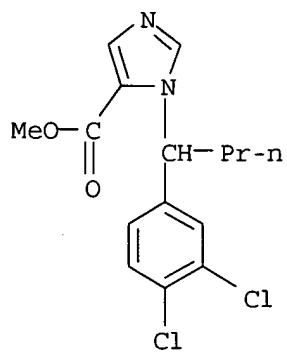
RN 112366-55-9 HCAPLUS

CN 1H-Imidazole-5-carboxylic acid, 1-[1-(3,4-dichlorophenyl)butyl]-, methyl ester, mononitrate (9CI) (CA INDEX NAME)

CM 1

CRN 112366-54-8

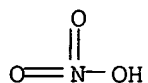
CMF C15 H16 Cl2 N2 O2



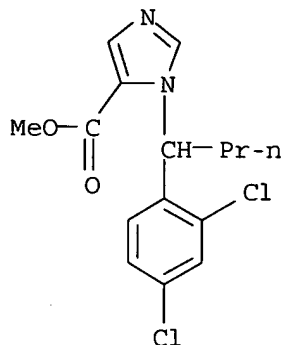
CM 2

CRN 7697-37-2

CMF H N O3



RN 112366-56-0 HCAPLUS
CN 1H-Imidazole-5-carboxylic acid, 1-[1-(2,4-dichlorophenyl)butyl]-, methyl ester (9CI) (CA INDEX NAME)

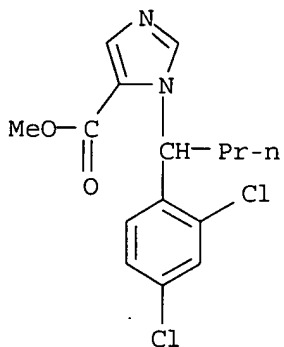


RN 112366-57-1 HCAPLUS
CN 1H-Imidazole-5-carboxylic acid, 1-[1-(2,4-dichlorophenyl)butyl]-, methyl ester, mononitrate (9CI) (CA INDEX NAME)

CM 1

CRN 112366-56-0

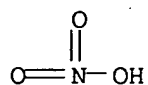
CMF C15 H16 Cl2 N2 O2



CM . 2

CRN 7697-37-2

CMF H N O3

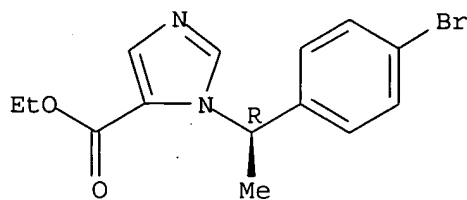


RN 112366-60-6 HCAPLUS
CN 1H-Imidazole-5-carboxylic acid, 1-[1-(4-bromophenyl)ethyl]-, ethyl ester,
(R)-, sulfate (1:1) (9CI) (CA INDEX NAME)

CM 1

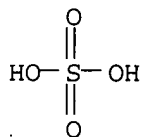
CRN 112366-59-3
CMF C14 H15 Br N2 O2

Absolute stereochemistry.

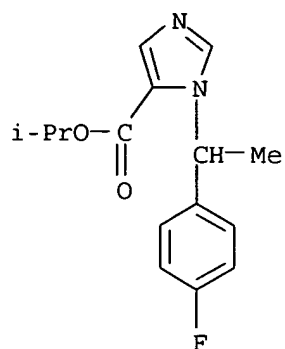


CM 2

CRN 7664-93-9
CMF H2 O4 S



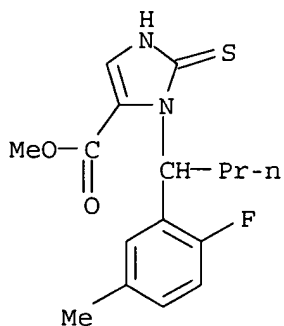
RN 112366-82-2 HCAPLUS
CN 1H-Imidazole-5-carboxylic acid, 1-[1-(4-fluorophenyl)ethyl]-,
1-methylethyl ester, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

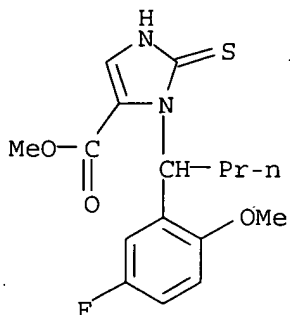
RN 112367-07-4 HCAPLUS

CN 1H-Imidazole-4-carboxylic acid, 3-[1-(2-fluoro-5-methylphenyl)butyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)



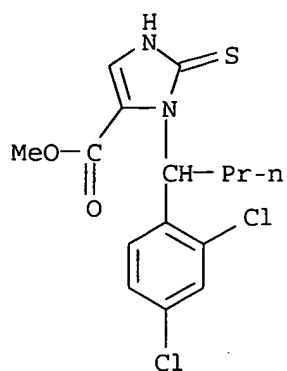
RN 112367-08-5 HCAPLUS

CN 1H-Imidazole-4-carboxylic acid, 3-[1-(5-fluoro-2-methoxyphenyl)butyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)



RN 112367-12-1 HCAPLUS

CN 1H-Imidazole-4-carboxylic acid, 3-[1-(2,4-dichlorophenyl)butyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)



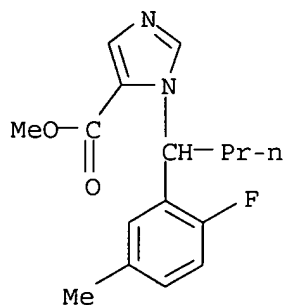
RN 112367-28-9 HCAPLUS

CN 1H-Imidazole-5-carboxylic acid, 1-[1-(2-fluoro-5-methylphenyl)butyl]-, methyl ester, mononitrate (9CI) (CA INDEX NAME)

CM 1

CRN 112367-27-8

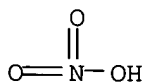
CMF C16 H19 F N2 O2



CM 2

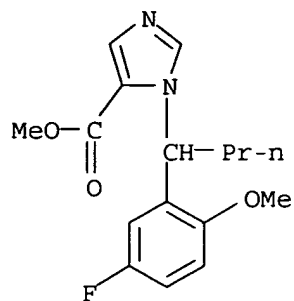
CRN 7697-37-2

CMF H N O3

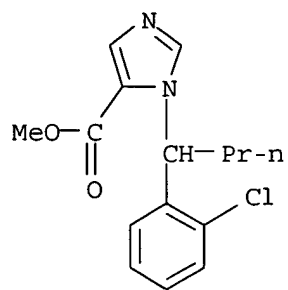


RN 112367-29-0 HCAPLUS

CN 1H-Imidazole-5-carboxylic acid, 1-[1-(5-fluoro-2-methoxyphenyl)butyl]-, methyl ester (9CI) (CA INDEX NAME)



RN 112367-32-5 HCAPLUS

CN 1H-Imidazole-5-carboxylic acid, 1-[1-(2-chlorophenyl)butyl]-, methyl ester
(9CI) (CA INDEX NAME)

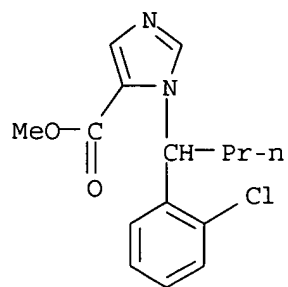
RN 112367-33-6 HCAPLUS

CN 1H-Imidazole-5-carboxylic acid, 1-[1-(2-chlorophenyl)butyl]-, methyl
ester, mononitrate (9CI) (CA INDEX NAME)

CM 1

CRN 112367-32-5

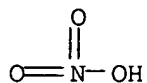
CMF C15 H17 Cl N2 O2



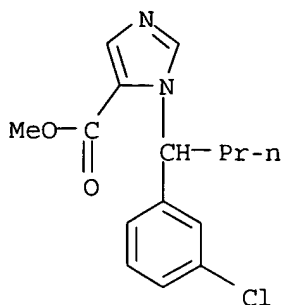
CM 2

CRN 7697-37-2

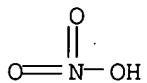
CMF H N O3



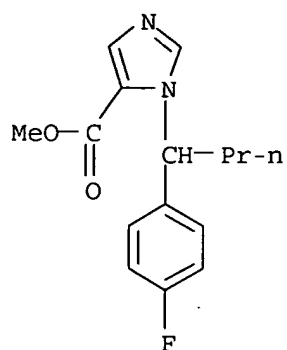
RN 112367-34-7 HCAPLUS
CN 1H-Imidazole-5-carboxylic acid, 1-[1-(3-chlorophenyl)butyl]-, methyl ester, mononitrate (9CI) (CA INDEX NAME)
CM 1
CRN 112366-35-5
CMF C15 H17 Cl N2 O2



CM 2
CRN 7697-37-2
CMF H N O3



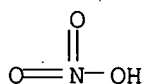
RN 112367-37-0 HCAPLUS
CN 1H-Imidazole-5-carboxylic acid, 1-[1-(4-fluorophenyl)butyl]-, methyl ester, mononitrate (9CI) (CA INDEX NAME)
CM 1
CRN 112367-36-9
CMF C15 H17 F N2 O2



CM 2

CRN 7697-37-2

CMF H N O3



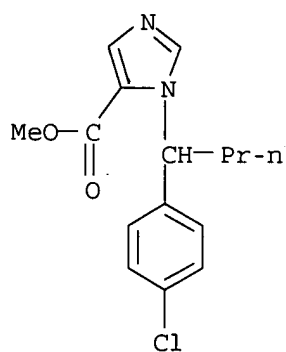
RN 112367-47-2 HCAPLUS

CN 1H-Imidazole-5-carboxylic acid, 1-[1-(4-chlorophenyl)butyl]-, methyl ester, mononitrate (9CI) (CA INDEX NAME)

CM 1

CRN 112367-46-1

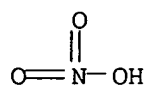
CMF C15 H17 Cl N2 O2



CM 2

CRN 7697-37-2

CMF H N O3

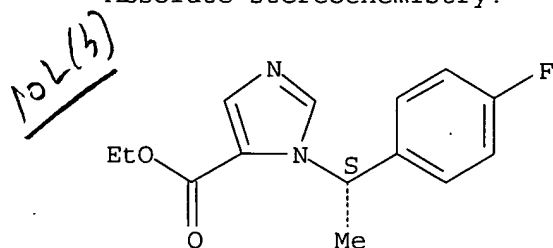


RN 112421-35-9 HCAPLUS
CN 1H-Imidazole-5-carboxylic acid, 1-[1-(4-fluorophenyl)ethyl]-, ethyl ester,
(S)-, sulfate (1:1) (9CI) (CA INDEX NAME)

CM 1

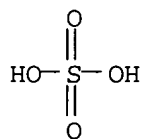
CRN 112421-34-8
CMF C14 H15 F N2 O2

Absolute stereochemistry.



CM 2

CRN 7664-93-9
CMF H2 O4 S

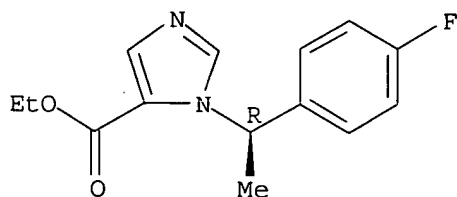


RN 112421-37-1 HCAPLUS
CN 1H-Imidazole-5-carboxylic acid, 1-[1-(4-fluorophenyl)ethyl]-, ethyl ester,
(R)-, sulfate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 112421-36-0
CMF C14 H15 F N2 O2

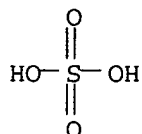
Absolute stereochemistry.



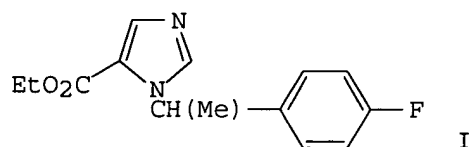
CM 2

CRN 7664-93-9

CMF H2 O4 S



L4 ANSWER 10 OF 15 HCAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1987:568686 HCAPLUS
 DOCUMENT NUMBER: 107:168686
 TITLE: Comparison of the effects of etomidate and its fluoro analog, R 8110, on plasma cortisol, 11 β -deoxycortisol, 17 α -hydroxyprogesterone and testosterone concentrations in dogs
 AUTHOR(S): De Coster, R.; Degryse, A. D. A. Y.; Van Dijk, P.; Ooms, L. A. A.; Lagerweij, E.
 CORPORATE SOURCE: Janssen Pharm., Beerse, Belg.
 SOURCE: Journal of Veterinary Pharmacology and Therapeutics (1987), 10(3), 227-32
 CODEN: JVPTD9; ISSN: 0140-7783
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB The effects of i.v. R 8110 (I), etomidate, and Ringer solution on cortisol biosynthesis by the adrenal gland was studied in male labradors. A tetracosactide challenge was carried out 30 min after the i.v. injection of 3 mg/kg of both drugs and after i.v. Ringer solution (1 mL/kg). Etomidate and R 8110 both suppressed the cortisol response tetracosactide almost completely and increased the plasma 11 β -deoxycortisol levels >20-fold. Maximal 11 β -deoxycortisol values were reached 120 min after R 8110, and \geq 300 min after etomidate. Plasma 17 α -hydroxyprogesterone and testosterone concns. did not differ between placebo and R 8110 treatment, but they decreased after etomidate. Thus, the effects of R 8110 on steroid biosynthesis in dogs are less pronounced than those of etomidate and are largely limited to a temporary inhibition of the 11 β -hydroxylase in the adrenal gland.

IT 109872-40-4, R8110

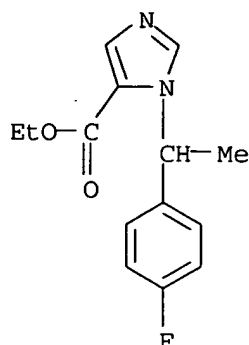
RL: BIOL (Biological study)

(steroids of blood plasma response to, etomidate in comparison with)

RN 109872-40-4 HCAPLUS

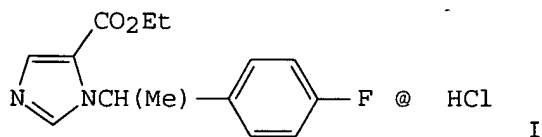
08/16/2005 10635294.trn

CN 1H-Imidazole-5-carboxylic acid, 1-[1-(4-fluorophenyl)ethyl]-, ethyl ester, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

L4 ANSWER 11 OF 15 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1987:526947 HCAPLUS
DOCUMENT NUMBER: 107:126947
TITLE: Clinical, cardiovascular and respiratory effects of R8110 in premedicated dogs
AUTHOR(S): Van Dijk, P.; Degryse, A. D.; Ooms, L.; Lagerweij, E.
CORPORATE SOURCE: Inst. Vet. Anaesth., State Univ. Utrecht, Utrecht, 3508 TD, Neth.
SOURCE: Journal of Veterinary Pharmacology and Therapeutics (1987), 10(2), 114-18
CODEN: JVPTD9; ISSN: 0140-7783
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



AB The clin., cardiovascular and respiratory effects after i.v. administration of R8110 (I) were studied in dogs. The clin. observations were made after doses of 3 and 4 mg/kg injected slowly i.v., whereas cardiovascular and respiratory studies were carried out at a dose of 3 mg/kg i.v. Induction and recovery were smooth and no significant side-effects were observed. The cardiovascular system was slightly influenced, but respiration was hardly affected. The effect of premedication on respiration and the cardiovascular system was hardly potentiated by R8110. Although there were significant changes in cardiovascular and biochem. parameters, all values remained within physiol. limits. R8110 appears to be a safe and reliable induction agent.

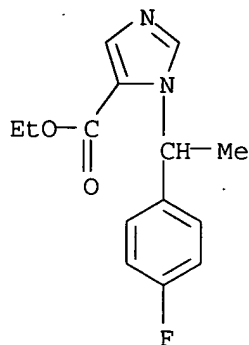
IT 109872-40-4

RL: PRP (Properties)

(anesthesia induction by and cardiovascular and respiratory effects of,
in premedicated dogs)

RN 109872-40-4 HCAPLUS

CN 1H-Imidazole-5-carboxylic acid, 1-[1-(4-fluorophenyl)ethyl]-, ethyl ester,
monohydrochloride (9CI) (CA INDEX NAME)



● HCl

L4 ANSWER 12 OF 15 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1987:489691 HCAPLUS

DOCUMENT NUMBER: 107:89691

TITLE: R 8110, a new short-acting hypnotic in dogs

AUTHOR(S): Van Dijk, P.; Degryse, A. D.; Ooms, L. A. A.;
Lagerweij, E.

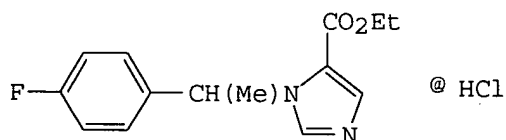
CORPORATE SOURCE: Univ. Vet. Anaesth., State Univ. Utrecht, Utrecht,
Neth.

SOURCE: Research in Veterinary Science (1987), 42(2), 200-3
CODEN: RVTSA9; ISSN: 0034-5288

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



@ HCl

I

AB The clin., respiratory and cardiovascular effects of i.v. injections of R 8110, (I) (3 or 4 mg/kg, i.v.) were studied in unpremedicated dogs. The drug proved to be a safe and reliable agent for induction and produced a short-lasting hypnosis and some analgesia. Both induction and recovery were smooth and rapid. Heart rate and systolic and diastolic blood pressure decreased 10 min after injection; the influence on arterial blood parameters was minimal.

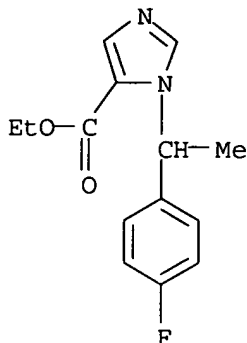
IT 109872-40-4

RL: BIOL (Biological study)

(cardiovascular and respiratory)

RN 109872-40-4 HCAPLUS

CN 1H-Imidazole-5-carboxylic acid, 1-[1-(4-fluorophenyl)ethyl]-, ethyl ester, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

L4 ANSWER 13 OF 15 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1976:59308 HCAPLUS

DOCUMENT NUMBER: 84:59308

TITLE: Synthesis of tritium-labeled etomidate and resolution into its enantiomers

AUTHOR(S): Heykants, J. J. P.; Knaeps, A. G.; Janssen, M. A. C.

CORPORATE SOURCE: Dep. Drug Metab., Janssen Pharm., Beerse, Belg.

SOURCE: Journal of Labelled Compounds (1975), 11(3), 401-7
CODEN: JLCAAI; ISSN: 0022-2135

DOCUMENT TYPE: Journal

LANGUAGE: English

GI For diagram(s), see printed CA Issue.

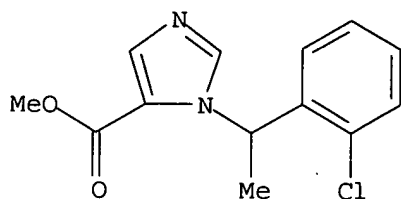
AB (+)-Etomidate-2-T[(+)-I] a short-acting hypnotic, was prepared by tritiation of the 2-chloro Et ester and subsequent hydrolysis and resolved into both enantiomers by salt formation with (R)-(+)- and (S)-(-)-PhCHMeNH₂.

IT 58294-52-3

RL: RCT (Reactant); RACT (Reactant or reagent)
(tritiation of)

RN 58294-52-3 HCAPLUS

CN 1H-Imidazole-5-carboxylic acid, 1-[1-(2-chlorophenyl)ethyl]-, methyl ester (9CI) (CA INDEX NAME)



L4 ANSWER 14 OF 15 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1966:447732 HCAPLUS
 DOCUMENT NUMBER: 65:47732
 ORIGINAL REFERENCE NO.: 65:8921e-h,8922a-b
 TITLE: Imidazolecarboxylates
 PATENT ASSIGNEE(S): Janssen Pharmaceutica N.V.
 SOURCE: 20 pp.
 DOCUMENT TYPE: Patent
 LANGUAGE: Unavailable
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
BE 662474		19651014	BE	
PRIORITY APPLN. INFO.:			US	19640416

GI For diagram(s), see printed CA Issue.

AB The title compds. (I) are used as hypnotics and anticonvulsants which do not influence breathing. They are prepared by oxidation with HNO₃ of 2-mercapto-5-imidazolecarboxylates, which in turn are prepared by condensation of N-acetyl-C-formylglycine enol ester (or alkali salts) with HCNS (Jones, CA 43, 3411a). Thus, a mixture of dl-1-phenylethylamine 132, Et₃N 110, HCON-Me₂ 100, and ClCH₂CO₂Et 133.5 parts is stirred overnight at 45° to give dl-N-(ethoxycarbonylmethyl)-1-phenylethylamine (II). II, HCO₂H 55.2, and xylene 480 parts is refluxed until the calculated amount of H₂O has separated to yield dl-N-formyl-N-(ethoxycarbonylmethyl)-1-phenylethylamine (III), b₃ 165-70°. The following dl-OHC NRCH₂CO₂Et were similarly prepared (R and b.p./mm. given): CH₂EtPh, 147-57°/2; CHPrPh, 185-8°/4; CHMeC₆H₄F-p, 185-92°/8; CHMeC₆H₄Cl-o, 154-60°/0.4; CHMeC₆H₄Cl-m, 160-6°/0.22; CHMeC₆H₄Cl-p, 170-3°/4; CHMeC₆H₄Br-p, 184-200/2; CHMeC₆H₄Me-p, 183-5°/4-5; CHMeC₆H₃Me₂-3,4, 153-6°/0.4; CHMeC₆H₄OMe-p, 190-2°/2; 2-thienylethyl, 145-8°/0.5; 2-pyridylethyl, 154-8°/0.4; 3-pyridylethyl, 174-9°/0.3-0.4; 4-pyridylethyl, 175-80°/0.6. A mixture of 29.9 parts 50% Na dispersion in paraffin oil and 300 parts tetrahydrofuran (IV) is stirred at 40°, MeOH 16 and IV 75 parts added, the mixture stirred 1 hr. at 40°, cooled to 10°, 144 parts III in 108 parts HCO₂Me added, stirred overnight at room temperature, concentrated in vacuo, and Et₂O 800 and H₂O 700 parts added.

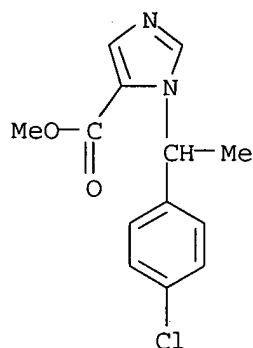
The aqueous layer is separated, diluted to 1000 parts, HCl 114 parts added, stirred 15

min. at 40°, KCNS 90 in H₂O 90 parts, added dropwise, stirred 3 hrs. at 40°, and overnight at room temperature to yield dl-1-(1-phenylethyl)-2-mercapto-5-(methoxycarbonyl)imidazole (V), m. 131-4°. Also prepared were the following dl-I (R₁ = SH, R₂ = Me) (Ar, R, and m.p. given): Ph, Me, 131-4°; Ph, Et, 209-10°; Ph, Pr, 175-7°; C₆H₄F-p, Me, 134-6°; C₆H₄Cl-o, Me, 183.5-6.5°; C₆H₄Cl-m, Me, 170-3°; C₆H₄Cl-p, Me, 161-2°; C₆H₄Br-p, Me, 157-61°; C₆H₄Me-p, Me, 163-5°; C₆H₃Me₂-3,4, Me, 136-8°; C₆H₄OMe-p, Me, 139.5-41°; 2-thienyl, Me, 162-4°; 2-pyridyl, Me, -; 3-pyridyl, Me, 201-2°; 4-pyridyl, Me, 181-4°; Ph, Me, 129.8-30.8°.

To a mixture of 80 parts HNO₃ (d. 1.37) and 200 parts H₂O is added 0.5 parts NaNO₂ at 25°, the temperature raised to 35° and 66 parts V added in portions to yield dl-1-(1-phenylethyl)-5-(methoxycarbonyl)imidazole-HCl, m. 173-4°. Also prepared were the following HCl salts of dl-I (R₁ = H) (Ar, R, R₂, and m.p. given): Ph, Me, Me, 173-4°; Ph, Et, Me, 167-8.5°; Ph, Pr, Me, 150.5-52°; C₆H₄F-p, Me, Me,

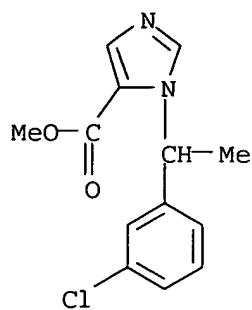
174-5.5°; C₆H₄Cl-o, Me, Me, 181-3°; C₆H₄Cl-m, Me, Me, 151-3.5°; C₆H₄Cl-p, Me, Me, 147-8°; C₆H₄Br-p, Me, Me, 137-9°; C₆H₄Me-p, Me, Me, 167-8°; C₆H₄Me₂-3,4, Me, Me, 166-7°; C₆H₄OMe-p, Me, Me, 129.5-30.5°; 2-thienyl, Me, Me, 135.5-38°; 2-pyridyl, Me, Me, 183.5-86.5°; 3-pyridyl, Me, Me, 178-89° (decomposition); 4-pyridyl, Me, Me, 79-80°; Ph, Me, Et, 142-2.8°; Ph, Me, H, 187-9°; Ph, Me, Cl, 161-263° (decomposition); Ph, Me, allyl, 134-6°; Ph, Me, propynyl, 92-3°; Ph, Me, Bu, 139-41°; Ph, Me, Am, 139-40°; Ph, Me, CH₂OMe, 112-14°; Ph, Me, Pr, 156-70°; Ph, Me, CH₂CH₂Cl, 83.5-85°; Ph, Et, H, 85-95°; Ph, Et, Et, 169-70.5°.

- IT **2852-45-1**, Imidazole-5-carboxylic acid, 1-(p-chloro- α -methylbenzyl)-, methyl ester, hydrochloride, (\pm)- **2852-47-3**, Imidazole-5-carboxylic acid, 1-(m-chloro- α -methylbenzyl)-, methyl ester, hydrochloride, (\pm)- **2852-49-5**, Imidazole-5-carboxylic acid, 1-(o-chloro- α -methylbenzyl)-, methyl ester, hydrochloride, (\pm)- **2852-51-9**, Imidazole-5-carboxylic acid, 1-(p-bromo- α -methylbenzyl)-, methyl ester, hydrochloride, (\pm)- **2881-39-2**, Imidazole-5-carboxylic acid, 1-(p-fluoro- α -methylbenzyl)-, methyl ester, hydrochloride, (\pm)- **91761-91-0**, Imidazole-5-carboxylic acid, 1-(p-bromo- α -methylbenzyl)-2-mercapto-, methyl ester, (\pm)- **91762-40-2**, Imidazole-5-carboxylic acid, 1-(o-chloro- α -methylbenzyl)-2-mercapto-, methyl ester, (\pm)- **91762-41-3**, Imidazole-5-carboxylic acid, 1-(p-chloro- α -methylbenzyl)-2-mercapto-, methyl ester, (\pm)- **92027-89-9**, Imidazole-5-carboxylic acid, 1-(p-fluoro- α -methylbenzyl)-2-mercapto-, methyl ester, (\pm)- **92849-54-2**, Imidazole-5-carboxylic acid, 1-(m-chloro- α -methylbenzyl)-2-mercapto-, methyl ester, (\pm)- (preparation of)
- RN 2852-45-1 HCAPLUS
- CN 1H-Imidazole-5-carboxylic acid, 1-[1-(4-chlorophenyl)ethyl]-, methyl ester, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

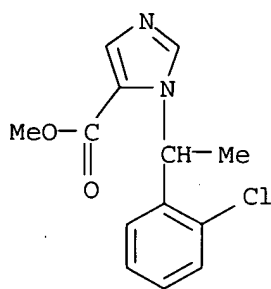
- RN 2852-47-3 HCAPLUS
- CN 1H-Imidazole-5-carboxylic acid, 1-[1-(3-chlorophenyl)ethyl]-, methyl ester, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 2852-49-5 HCAPLUS

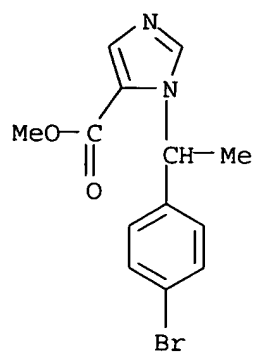
CN 1H-Imidazole-5-carboxylic acid, 1-[1-(2-chlorophenyl)ethyl]-, methyl ester, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 2852-51-9 HCAPLUS

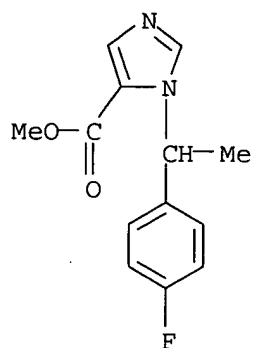
CN 1H-Imidazole-5-carboxylic acid, 1-[1-(4-bromophenyl)ethyl]-, methyl ester, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 2881-39-2 HCAPLUS

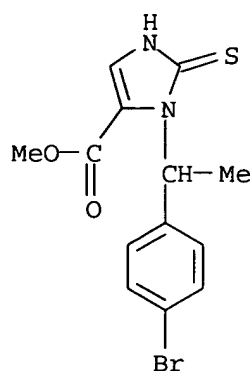
CN 1H-Imidazole-5-carboxylic acid, 1-[1-(4-fluorophenyl)ethyl]-, methyl ester, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

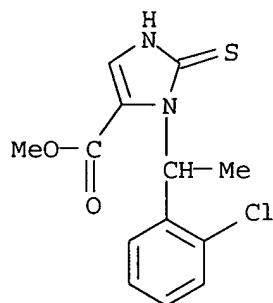
RN 91761-91-0 HCAPLUS

CN 1H-Imidazole-4-carboxylic acid, 3-[1-(4-bromophenyl)ethyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)



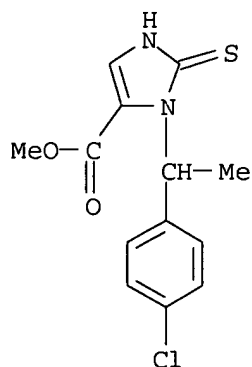
RN 91762-40-2 HCAPLUS

CN 1H-Imidazole-4-carboxylic acid, 3-[1-(2-chlorophenyl)ethyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)



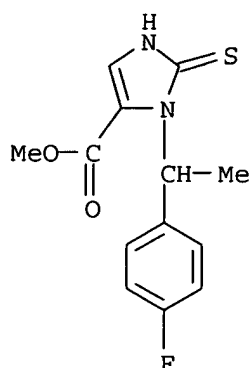
RN 91762-41-3 HCAPLUS

CN 1H-Imidazole-4-carboxylic acid, 3-[1-(4-chlorophenyl)ethyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)



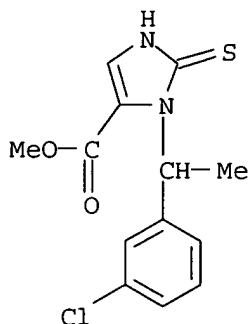
RN 92027-89-9 HCAPLUS

CN 1H-Imidazole-4-carboxylic acid, 3-[1-(4-fluorophenyl)ethyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)



RN 92849-54-2 HCAPLUS

CN 1H-Imidazole-4-carboxylic acid, 3-[1-(3-chlorophenyl)ethyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)



L4 ANSWER 15 OF 15 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1965:58908 HCAPLUS

DOCUMENT NUMBER: 62:58908

ORIGINAL REFERENCE NO.: 62:10428d-e

TITLE: DL-1-(1-(Arylalkyl)imidazole-5-carboxylate esters. A novel type of hypnotic agents

AUTHOR(S): Godefroi, Erik F.; Janssen, Paul A. J.; van der Eycken, Cyriel A. M.; van Heertum, Albert H. M. T.; Niemegeers, Carlos J. E.

CORPORATE SOURCE: Janssen Pharm., Beerse, Belg.

SOURCE: Journal of Medicinal Chemistry (1965), 8(2), 220-3
CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: Journal

LANGUAGE: English

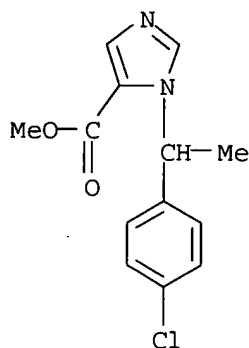
AB A number of 1-substituted imidazole-5-carboxylic acid esters (I) have been synthesized. Many of these are extremely potent, rapid, and short-acting hypnotic agents in rats.

IT **2852-45-1**, Imidazole-5-carboxylic acid, 1-(p-chloro- α -methylbenzyl)-, methyl ester, hydrochloride **2852-47-3**, Imidazole-5-carboxylic acid, 1-(m-chloro- α -methylbenzyl)-, methyl ester, hydrochloride **2852-49-5**, Imidazole-5-carboxylic acid, 1-(o-chloro- α -methylbenzyl)-, methyl ester, hydrochloride **2852-51-9**, Imidazole-5-carboxylic acid, 1-(p-bromo- α -methylbenzyl)-, methyl ester, hydrochloride **2881-39-2**, Imidazole-5-carboxylic acid, 1-(p-fluoro- α -methylbenzyl)-, methyl

ester, hydrochloride **91761-91-0**, Imidazole-5-carboxylic acid, 1-(p-bromo- α -methylbenzyl)-2-mercapto-, methyl ester
91762-40-2, Imidazole-5-carboxylic acid, 1-(o-chloro- α -methylbenzyl)-2-mercapto-, methyl ester **91762-41-3**, Imidazole-5-carboxylic acid, 1-(p-chloro- α -methylbenzyl)-2-mercapto-, methyl ester **92027-89-9**, Imidazole-5-carboxylic acid, 1-(p-fluoro- α -methylbenzyl)-2-mercapto-, methyl ester **92849-54-2**, Imidazole-5-carboxylic acid, 1-(m-chloro- α -methylbenzyl)-2-mercapto-, methyl ester
(preparation of)

RN 2852-45-1 HCAPLUS

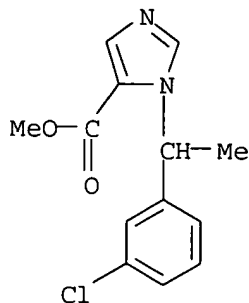
CN 1H-Imidazole-5-carboxylic acid, 1-[1-(4-chlorophenyl)ethyl]-, methyl ester, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 2852-47-3 HCAPLUS

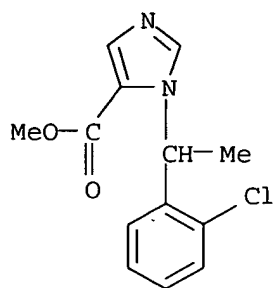
CN 1H-Imidazole-5-carboxylic acid, 1-[1-(3-chlorophenyl)ethyl]-, methyl ester, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 2852-49-5 HCAPLUS

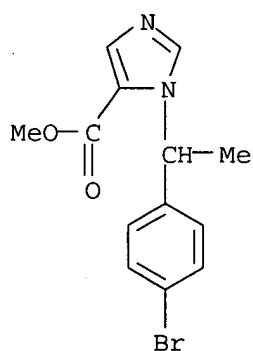
CN 1H-Imidazole-5-carboxylic acid, 1-[1-(2-chlorophenyl)ethyl]-, methyl ester, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 2852-51-9 HCAPLUS

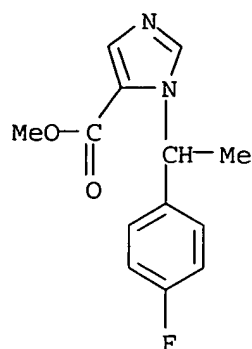
CN 1H-Imidazole-5-carboxylic acid, 1-[1-(4-bromophenyl)ethyl]-, methyl ester, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 2881-39-2 HCAPLUS

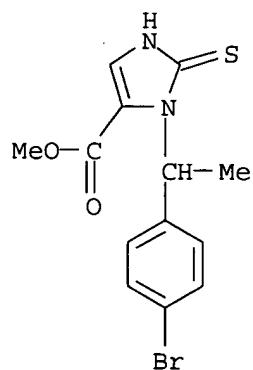
CN 1H-Imidazole-5-carboxylic acid, 1-[1-(4-fluorophenyl)ethyl]-, methyl ester, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

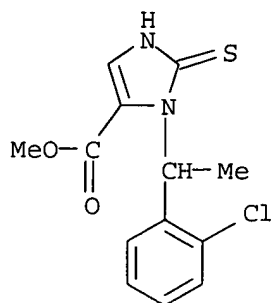
RN 91761-91-0 HCAPLUS

CN 1H-Imidazole-4-carboxylic acid, 3-[1-(4-bromophenyl)ethyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)



RN 91762-40-2 HCAPLUS

CN 1H-Imidazole-4-carboxylic acid, 3-[1-(2-chlorophenyl)ethyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)

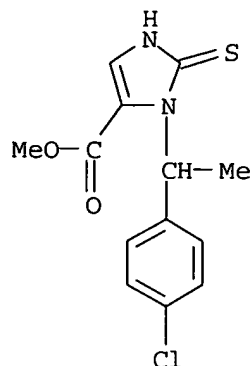


RN 91762-41-3 HCAPLUS

CN 1H-Imidazole-4-carboxylic acid, 3-[1-(4-chlorophenyl)ethyl]-2,3-dihydro-2-

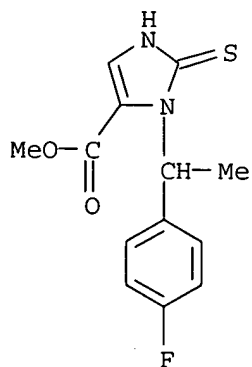
08/16/2005 10635294.trn

thioxo-, methyl ester (9CI) (CA INDEX NAME)



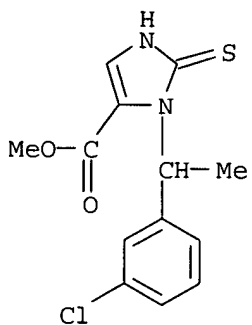
RN 92027-89-9 HCAPLUS

CN 1H-Imidazole-4-carboxylic acid, 3-[1-(4-fluorophenyl)ethyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)



RN 92849-54-2 HCAPLUS

CN 1H-Imidazole-4-carboxylic acid, 3-[1-(3-chlorophenyl)ethyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)



=> d 16 ibib abs hitstr tot

08/16/2005 10635294.trn

YOU HAVE REQUESTED DATA FROM FILE 'REGISTRY' - CONTINUE? (Y)/N:n

=> d his

(FILE 'HOME' ENTERED AT 09:22:09 ON 16 AUG 2005)

FILE 'REGISTRY' ENTERED AT 09:22:20 ON 16 AUG 2005

L1 STRUCTURE UPLOADED

L2 7 S L1

L3 95 S L1 SSS FULL

FILE 'HCAPLUS' ENTERED AT 09:22:48 ON 16 AUG 2005

L4 15 S L3

FILE 'REGISTRY' ENTERED AT 09:25:22 ON 16 AUG 2005

L5 STRUCTURE UPLOADED

L6 1 S L5

L7 19 S L5 SSS FULL

FILE 'HCAPLUS' ENTERED AT 09:25:53 ON 16 AUG 2005

L8 6 S L7

=> d l8 ibib abs hitstr tot

L8 ANSWER 1 OF 6 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2005:123220 HCAPLUS

DOCUMENT NUMBER: 142:198079

TITLE: Preparation of radiolabeled 1-(phenylethyl)imidazole-5-carboxylic acid ester derivatives

INVENTOR(S): Zolle, Ilse; Hammerschmidt, Friedrich

PATENT ASSIGNEE(S): Austria

SOURCE: U.S. Pat. Appl. Publ., 15 pp.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005033060	A1	20050210	US 2003-635294	20030806
PRIORITY APPLN. INFO.:			US 2003-635294	20030806
OTHER SOURCE(S):	MARPAT	142:198079		
GI				

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Halogenated carboxylic ester derivs. of phenylethylimidazole (I) [R1 = linear or branched C1-4 alkyl which is optionally substituted with a halogen selected from the groups consisting of F, Cl, I or Br; R2 = C1-2 alkyl; X = a nonradioactive or a radioactive halogen] or (II) [X = a nonradioactive or radioactive halogen selected from the group consisting of I, Br, and F; X = a radioactive halogen selected from the group consisting of 123I, 124I, 131I, 76Br, 82Br or 18F] are prepared via coupling of (S)-secondary alc. (III) (R2, X = same as above) with

imidazolecarboxylate ester (IV) (R1 = same as above). Radio-halogenated forms of these compds. are ideally suited for positron-imaging of the adrenal glands, as it is known that these compds. demonstrate a selective and high rate of accumulation in the adrenals. The method of preparing these derivs. proceeds by the conversion of a stable, non-radioactive intermediate having trialkylstannyl leaving groups (V) [R1, R2 = same as above; L = an alkylstannyl group selected from the group consisting of trimethylstannyl, triethylstannyl, tri-n-propylstannyl and tri-n-butylstannyl] and (VI) (R1, R2 = same as above). These intermediates are efficiently converted to the corresponding halogenated forms by substitution of the trialkylstannyl group with the halogen or radiohalogen. Thus, 4-iodoacetophenone was reduced by DIBAL in toluene/Et2O at -78° to give 86% 1-(4-iodophenyl)ethanol which was esterified by chloroacetic anhydride in the presence of pyridine in CH2Cl2 at 0° for 2 h to give 91% 1-(4-iodophenyl)ethyl chloroacetate (VII). VII underwent enzymic hydrolysis in the presence of lipase SAM II in a mixture of tert-Bu Me ether and phosphate buffer at 0° for 2 h while keeping pH at 7.0 by adding 0.5 N aqueous NaOH solution to give 43% (R)-1-(4-iodophenyl)ethanol (98% ee) and 44% (S)-1-(4-iodophenyl)ethyl chloroacetate (>98% ee) (VIII). VIII was coupled with Me 3H-imidazole-4-carboxylate using triphenylphosphine and di(tert-butyl) azocarbonylate in THF at -30° to 0° over 2.5 h to give 67% (R)-(+)-Me 3-[1-(4-iodophenyl)ethyl]-3H-imidazole-4-carboxylate (99% ee) which was refluxed with hexamethyltin in toluene at 135° for 17 h to give 96% (R)-(+)-Me 3-[1-[4-(trimethylstannyl)phenyl]ethyl]-3H-imidazole-4-carboxylate (IX). IX (30 µg) was reacted with [131I]iodide in 10-20 µL 0.05 N aqueous NaOH solution; 15 µL aqueous chloramine-T solution

(1 mg/mL), and 6 µL 1 N aqueous HCl solution at room temperature for 1 min to give (R)-(+)-Me 3-[1-(4-[131I]iodophenyl)ethyl]-3H-imidazole-4-carboxylate (131I-MTO), i.e. II (R1 = R2 = Me, X = 131I).

IT **813466-09-0P**

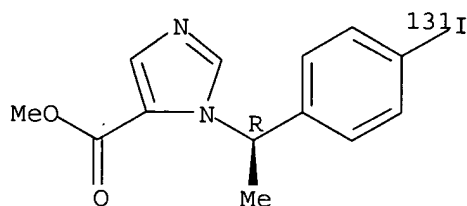
RL: BSU (Biological study, unclassified); DGN (Diagnostic use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of radiolabeled (phenylethyl)imidazolecarboxylic acid ester derivs. as positron-emission imaging agents for adrenal glands)

RN 813466-09-0 HCAPLUS

CN 1H-Imidazole-5-carboxylic acid, 1-[(1R)-1-[4-(iodo-131I)phenyl]ethyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



IT **813466-05-6P**, (R)-(+)-Methyl 3-[1-(4-Iodophenyl)ethyl]-3H-imidazole-4-carboxylate

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

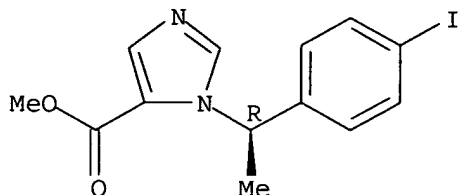
(preparation of radiolabeled (phenylethyl)imidazolecarboxylic acid ester derivs. as positron-emission imaging agents for adrenal glands)

08/16/2005 10635294.trn

RN 813466-05-6 HCAPLUS

CN 1H-Imidazole-5-carboxylic acid, 1-[(1R)-1-(4-iodophenyl)ethyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



L8 ANSWER 2 OF 6 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2005:74646. HCAPLUS

DOCUMENT NUMBER: 142:280123

TITLE: 2-Mercaptoimidazoles, a new class of potent CCR2 antagonists

AUTHOR(S): Van Lommen, Guy; Doyon, Julien; Coesemans, Erwin; Boeckx, Staf; Cools, Marina; Buntinx, Mieke; Hermans, Bart; Van Wauwe, Jean

CORPORATE SOURCE: Inflammation Research, Johnson and Johnson Pharmaceutical Research and Development, Beerse, B-2340, Belg.

SOURCE: Bioorganic & Medicinal Chemistry Letters (2005), 15(3), 497-500

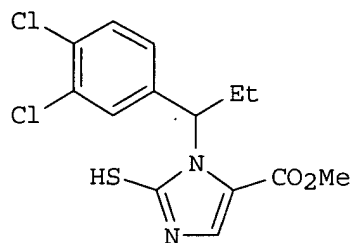
CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



AB The synthesis and SAR of a class of CCR2 antagonists based on a 2-mercaptoimidazole scaffold, e.g., I. The initial lead compound was optimized to the corresponding optical active 3,4-disubstituted analogs, which have IC50 values in the MCP-1 induced Ca-flux below 0.01 μ M.

IT 742107-81-9P 742107-82-0P

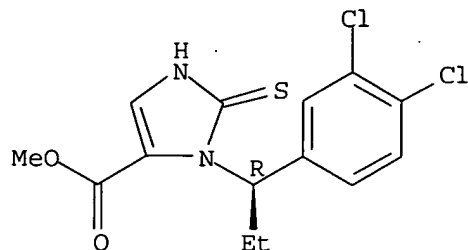
RL: PAC (Pharmacological activity); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent).

(stereoselective preparation, CCR2 antagonistic activity, and structure-activity relationship of mercaptoimidazoles using asym. addition and heterocyclization as the key steps)

RN 742107-81-9 HCAPLUS

CN 1H-Imidazole-4-carboxylic acid, 3-[(1R)-1-(3,4-dichlorophenyl)propyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)

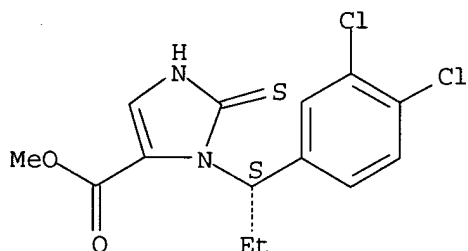
Absolute stereochemistry. Rotation (+).



RN 742107-82-0 HCAPLUS

CN 1H-Imidazole-4-carboxylic acid, 3-[(1S)-1-(3,4-dichlorophenyl)propyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



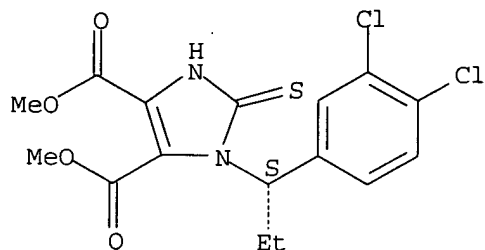
IT 847448-27-5P 847448-28-6P 847448-29-7P

RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(stereoselective preparation, CCR2 antagonistic activity, and structure-activity relationship of mercaptoimidazoles using asym. addition and heterocyclization as the key steps)

RN 847448-27-5 HCAPLUS

CN 1H-Imidazole-4,5-dicarboxylic acid, 1-[(1S)-1-(3,4-dichlorophenyl)propyl]-2,3-dihydro-2-thioxo-, dimethyl ester (9CI) (CA INDEX NAME)

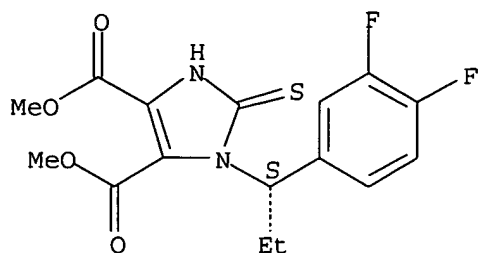
Absolute stereochemistry.



RN 847448-28-6 HCAPLUS

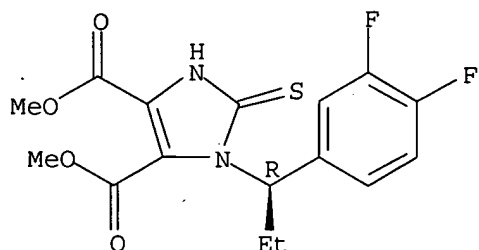
CN 1H-Imidazole-4,5-dicarboxylic acid, 1-[(1S)-1-(3,4-difluorophenyl)propyl]-2,3-dihydro-2-thioxo-, dimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 847448-29-7 HCAPLUS
 CN 1H-Imidazole-4,5-dicarboxylic acid, 1-[(1R)-1-(3,4-difluorophenyl)propyl]-2,3-dihydro-2-thioxo-, dimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 3 OF 6 HCAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 2004:686636 HCAPLUS
 DOCUMENT NUMBER: 142:88850
 TITLE: [123/131I]iodometomidate as a radioligand for functional diagnosis of adrenal disease: Synthesis, structural requirements and biodistribution
 AUTHOR(S): Schirbel, A.; Zolle, I.; Hammerschmidt, F.; Berger, M. L.; Schiller, D.; Kwaeternik, H.; Reiners, Chr.
 CORPORATE SOURCE: Department of Nuclear Medicine, University of Wuerzburg, Germany
 SOURCE: Radiochimica Acta (2004) 92(4-6), 297-303
 CODEN: RAACAP; ISSN: 0033-8230
 PUBLISHER: Oldenbourg Wissenschaftsverlag GmbH
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Metomidate [(R)-1-(1-phenylethyl)-1H-imidazole-5-carboxylic acid Me ester] (MTO, 1, Fig. 1) is a potent and selective inhibitor of the cytochrome P 450 enzyme system in the adrenal cortex. Labeled in the 4-position with radioiodine, (R)-4-[131I]iodometomidate, 2, [131I]IMTO has been evaluated by in-vitro studies and also ex-vivo in rats. [131I]IMTO was synthesized by oxidative radioiododestannylation using a suitable precursor which was prepared by a new stereoselective synthesis. Optimization of the labeling reaction was performed by systematic variation of the most important reaction parameters. Under optimum reaction conditions, a labeling yield of 95% was obtained. In-vitro-stability of the tracer was studied over 8

days, indicating slow deiodination (0.27%/h). Displacement studies using [^{131}I]IMTO and rat adrenal membranes revealed the structural requirements for high affinity binding, namely an intact ester group and (R)-configuration of the radioligand. Pharmacokinetic studies in rats showed fast accumulation of [^{131}I]IMTO in the adrenals (approx. 10% ID/g tissue) with an activity plateau for 2 h. Metabolic degradation was indicated by a steady increase of renal activity up to 4 h post injection. Based on target to non-target ratios the highest contrast for imaging of the adrenals was observed between 30 and 60 min post injection of [^{131}I]IMTO. We conclude that SPECT using [^{123}I]IMTO will be a promising method for the characterization of adrenal incidentalomas.

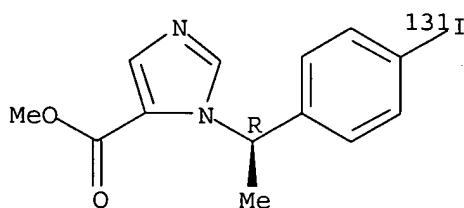
IT **813466-09-0**

RL: BSU (Biological study, unclassified); BIOL (Biological study) (synthesis, structural requirements and biodistribution of [$^{123}/^{131}\text{I}$]iodometomidate as a radioligand for functional diagnosis of adrenal disease)

RN 813466-09-0 HCAPLUS

CN 1H-Imidazole-5-carboxylic acid, 1-[(1R)-1-[4-(iodo- ^{131}I)phenyl]ethyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



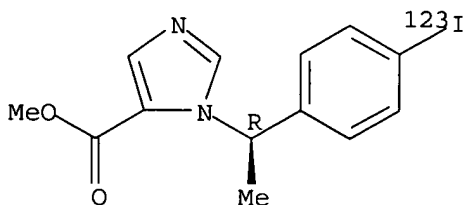
IT **813466-08-9P**

RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation) (synthesis, structural requirements and biodistribution of [$^{123}/^{131}\text{I}$]iodometomidate as a radioligand for functional diagnosis of adrenal disease)

RN 813466-08-9 HCAPLUS

CN 1H-Imidazole-5-carboxylic acid, 1-[(1R)-1-[4-(iodo- ^{123}I)phenyl]ethyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



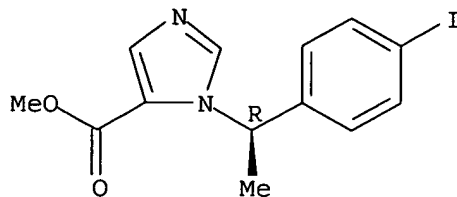
IT **813466-05-6P**

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation) (synthesis, structural requirements and biodistribution of [$^{123}/^{131}\text{I}$]iodometomidate as a radioligand for functional diagnosis of adrenal disease)

RN 813466-05-6 HCAPLUS

CN 1H-Imidazole-5-carboxylic acid, 1-[(1R)-1-(4-iodophenyl)ethyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 4 OF 6 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:675729 HCAPLUS

DOCUMENT NUMBER: 141:207206

TITLE: Preparation of mercaptoimidazoles as CCR2 receptor antagonists for the treatment of inflammatory disease
INVENTOR(S): Van Lommen, Guy Rosalia Eugeen; Doyon, Julien Georges Pierre-Olivier; Van Wauwe, Jean Pierre Frans; Cools, Marina Lucie Louise; Coesemans, Erwin

PATENT ASSIGNEE(S): Janssen Pharmaceutica N.V., Belg.

SOURCE: PCT Int. Appl., 64 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004069809	A1	20040819	WO 2003-EP301038	20030203
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
WO 2004069810	A1	20040819	WO 2004-EP957	20040130
W:	AE, AE, AG, AL, AL, AM, AM, AM, AT, AT, AU, AZ, AZ, BA, BB, BG, BG, BR, BR, BW, BY, BY, BZ, BZ, CA, CH, CN, CN, CO, CO, CR, CR, CU, CU, CZ, CZ, DE, DE, DK, DK, DM, DZ, EC, EC, EE, EE, EG, ES, ES, FI, FI, GB, GD, GE, GE, GH, GM, HR, HR, HU, HU, ID, IL, IN, IS, JP, JP, KE, KE, KG, KG, KP, KP, KP, KR, KR, KZ, KZ, KZ, LC, LK, LR, LS, LS, LT, LU, LV, MA, MD, MD, MG, MK, MN, MW, MX, MX, MZ, MZ, NA, NI			
RW:	BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			

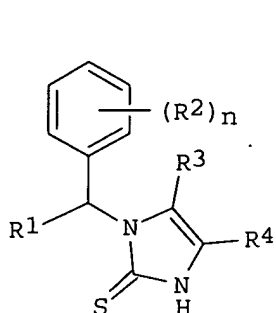
PRIORITY APPLN. INFO.:

WO 2003-EP1038

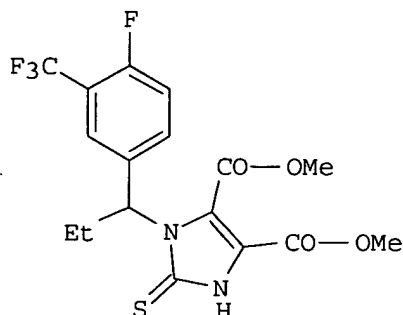
A 20030203

OTHER SOURCE(S): MARPAT 141:207206

GI



I



II

AB The invention relates to mercaptoimidazoles of formula I, N-oxides, pharmaceutically acceptable addition salts, quaternary amines and stereochem. isomeric forms thereof, wherein R1 is H, (cyclo)alkyl, (hetero)aryl; R2 is halo, alkyl(oxy/thio), polyhaloalkyl(oxy), cyano, aminocarbonyl, (di)(alkyl)amino, nitro, aryl(oxy); R3 and R4 are H, cyano, (hydroxy)alkyl, C(O)OR5, C(O)NR6aR6b, S(O)2NR6aR6b, C(O)R7; R5 is a defined carbon or N-heterocyclic ester group; R6a, R6b is H, alkyl, (di)(alkyl)amino(alkyl), arylamino; or NR6aR6b is a N-heterocycle; R7 is H, alk(en/yn)yl, aryl, certain substituted alkyls; n is 1-5, etc., with some limitations. The compds. have been synthesized as CCR2 receptor antagonists and found useful for the treatment and prevention of diseases, such as inflammation, which are mediated through activation of the CCR2 receptor, particularly CCR2B receptor. The invention also relates to processes for preparing the compds. and pharmaceutical compns. comprising them. Thus, compound II was prepared from 1-[4-fluoro-3-(trifluoromethyl)phenyl]-1-propanone via oxime formation, reduction, N-alkylation with Me bromoacetate, formylation and finally cyclocondensation with (CO2Me)2 and KSCN. The synthesized compds. showed inhibition of MCP-1 induced Ca-flux in human THP-1 cells with pIC50 5.6-8.2 (pIC50 = -log IC50).

IT 742107-81-9P 742107-82-0P

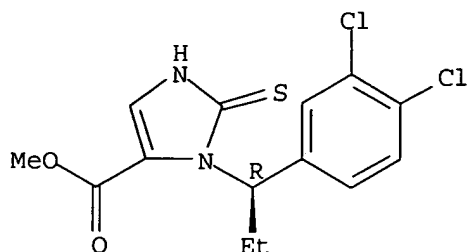
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(receptor antagonist; preparation of mercaptoimidazoles as CCR2 receptor antagonists for the treatment of inflammatory disease)

RN 742107-81-9 HCAPLUS

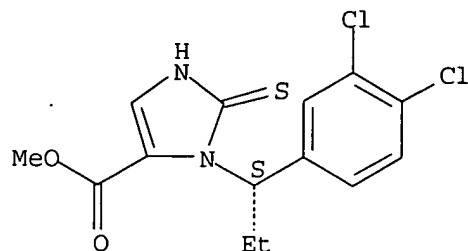
CN 1H-Imidazole-4-carboxylic acid, 3-[(1R)-1-(3,4-dichlorophenyl)propyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

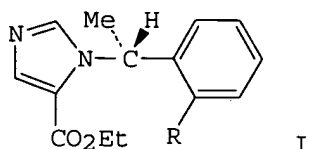


RN 742107-82-0 HCAPLUS
 CN 1H-Imidazole-4-carboxylic acid, 3-[(1S)-1-(3,4-dichlorophenyl)propyl]-2,3-dihydro-2-thioxo-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



L8 ANSWER 5 OF 6 HCAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1988:167377 HCAPLUS
 DOCUMENT NUMBER: 108:167377
 TITLE: Synthesis of (R)-(+)-3H-etomidate
 AUTHOR(S): Janssen, Cor G. M.; Thijssen, Jos B. A.; Verluyten, Willy L. M.; Heykants, Jozef J. P.
 CORPORATE SOURCE: Dep. Drug Metab. Pharmacokinet., Janssen Pharm., Beerse, B-2340, Belg.
 SOURCE: Journal of Labelled Compounds and Radiopharmaceuticals (1987), 24(8), 909-18
 CODEN: JLCRD4; ISSN: 0362-4803
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 108:167377
 GI



AB Etomidate, (R)-(+)-ethyl-1-(1-phenylethyl)-1H-imidazole-5-carboxylate (I, R = H) is a short-acting hypnotic. A new synthesis, featuring optical resolution on a non-radioactive precursor and introduction of the tritium label by reductive dehalogenation of I (R = Br) is described. I (R = T)

was obtained at a specific activity of 3.77 Ci/mmol and a 99.9% purity.

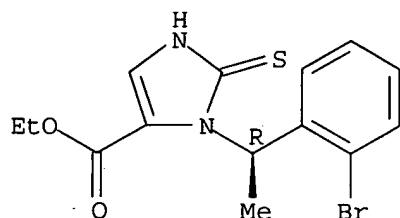
IT 112366-36-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and desulfurization of, with sodium nitrite)

RN 112366-36-6 HCAPLUS

CN 1H-Imidazole-4-carboxylic acid, 3-[1-(2-bromophenyl)ethyl]-2,3-dihydro-2-thioxo-, ethyl ester, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 112366-50-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 112366-50-4 HCAPLUS

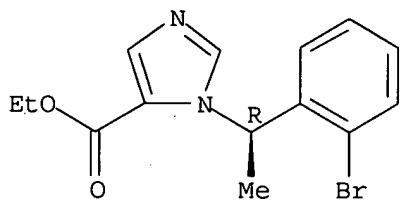
CN 1H-Imidazole-5-carboxylic acid, 1-[1-(2-bromophenyl)ethyl]-, ethyl ester, (R)-, sulfate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 112366-49-1

CMF C14 H15 Br N2 O2

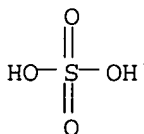
Absolute stereochemistry.



CM 2

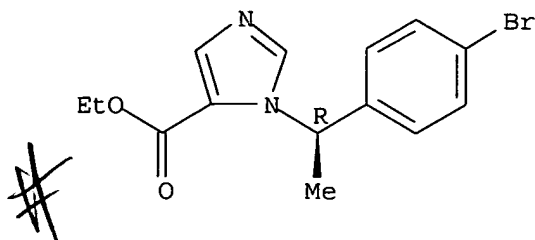
CRN 7664-93-9

CMF H2 O4 S



IT 112366-49-1P

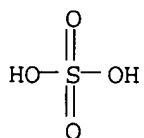
Absolute stereochemistry.



CM 2

CRN 7664-93-9

CMF H2 O4 S



RN 112421-35-9 HCAPLUS

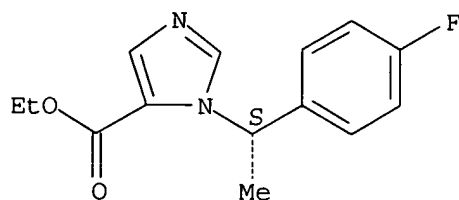
CN 1H-Imidazole-5-carboxylic acid, 1-[1-(4-fluorophenyl)ethyl]-, ethyl ester, (S)-, sulfate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 112421-34-8

CMF C14 H15 F N2 O2

Absolute stereochemistry.



CM 2

CRN 7664-93-9

CMF H2 O4 S

